The Unscrambler

Program Operation

By CAMO Software AS

CAMO

www.camo.com

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Software Version

This manual is up to date for version 9.6 of The Unscrambler®.

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Installation and Configuration

In this chapter, you will learn about system requirements for installing and running The Unscrambler, installation procedure and system configuration after installation.

The Unscrambler® satisfies the FDA's requirements for 21 CFR Part 11 compliance.

System Requirements

This section presents hardware and software requirements for installing and running The Unscrambler.

Hardware Requirements

We recommend that you use at least a Pentium PC running at 100 MHz or more. Memory space is an important issue, at least 16 MB of RAM should be available, preferably 32 MB. Using a more powerful PC improves performance significantly and is advisable if your data tables are large.

Software Requirements

The Unscrambler software is written for the Windows 95, Windows 98, Windows NT (3.51 or later), Windows 2000 and Windows XP operating systems.

The Program does not run on Windows 3.x or Windows for Workgroups platforms.

Standalone Installation (1-User License Desktop Installation)

Installing The Unscrambler Standalone is a straightforward procedure in five steps:

1. Download of The Unscrambler
2. Installation of The Unscrambler
3. Request of an Unscrambler Activation Key
4. Activation of The Unscrambler
5. Definition of user name and password in supervisor login mode

A detailed description of each of these steps is given below.

Downloading The Unscrambler

1. Download The Unscrambler Standalone installer from www.camo.com and save it into a Temp folder.

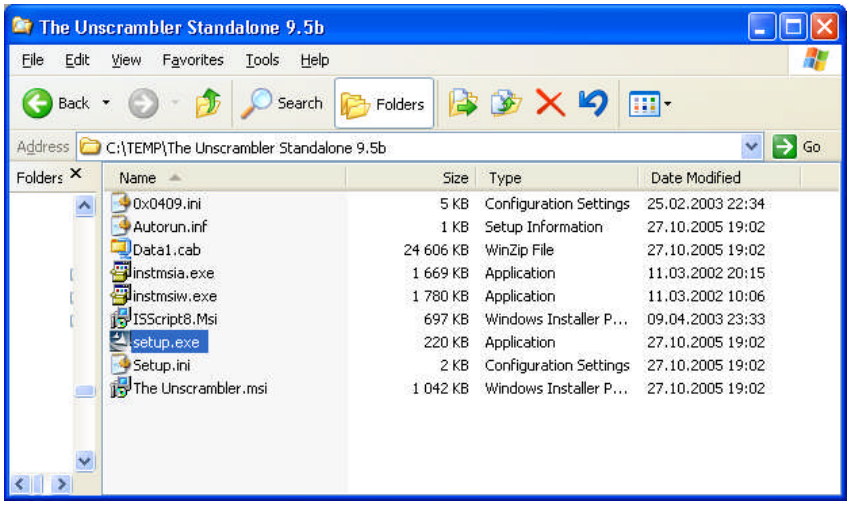
2. Extract the file. A folder **The Unscrambler Standalone** is created.

Installing The Unscrambler

If you are upgrading to a new version, it is recommended to uninstall your previous Unscrambler installation prior to installing the new one.

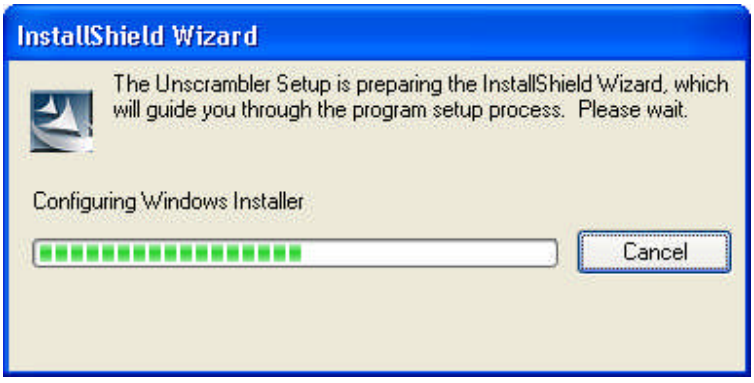
Un-installing your former Unscrambler version will remove the program files only; all your Unscrambler data files and model files will be preserved.

3. If you have downloaded The Unscrambler from Camo's website, double-click on file **setup.exe** file found in folder **The Unscrambler Standalone** to start the installation.

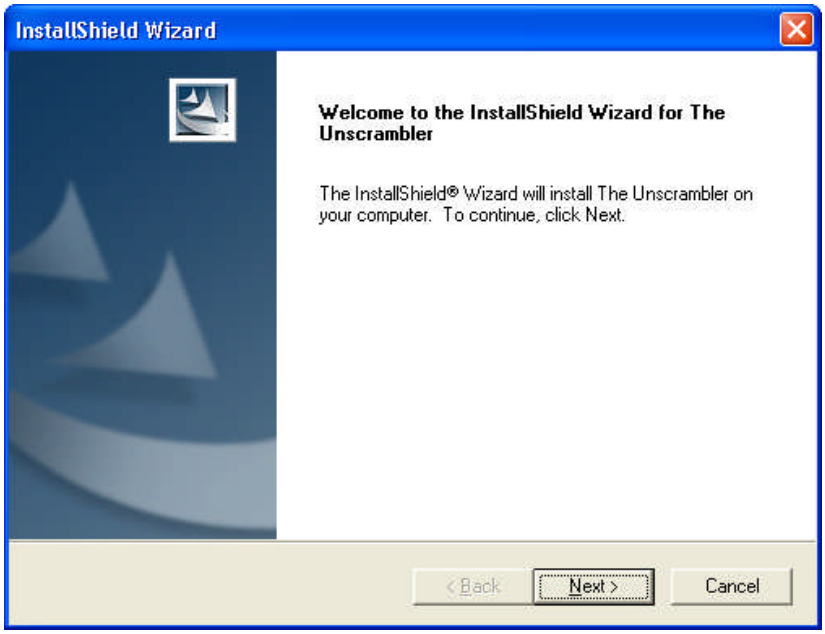

The Unscrambler Standalone 9.5b
File Edit View Favorites Tools Help
Back Search Folders
Address C:\TEMP\The Unscrambler Standalone 9.5b
Go
Folders
Name Size Type Date Modified
0x0409.ini 5 KB Configuration Settings 25.02.2003 22:34
Autorun.inf 1 KB Setup Information 27.10.2005 19:02
Data1.cab 24 606 KB WinZip File 27.10.2005 19:02
instmsia.exe 1 669 KB Application 11.03.2002 20:15
instmsiw.exe 1 780 KB Application 11.03.2002 10:06
ISScript8.Msi 697 KB Windows Installer P... 09.04.2003 23:33
setup.exe 220 KB Application 27.10.2005 19:02
Setup.ini 2 KB Configuration Settings 27.10.2005 19:02
The Unscrambler.msi 1 042 KB Windows Installer P... 27.10.2005 19:02

If you have received The Unscrambler installer on CD-ROM, place the CD in your CD player.

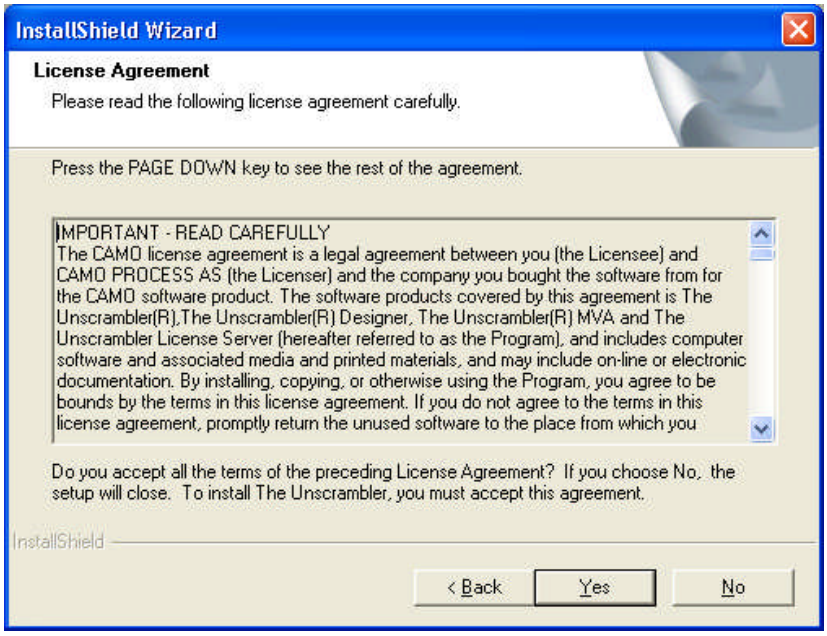
4. An **InstallShield Wizard** dialog opens


InstallShield Wizard
The Unscrambler Setup is preparing the InstallShield Wizard, which will guide you through the program setup process. Please wait.
Configuring Windows Installer
Cancel

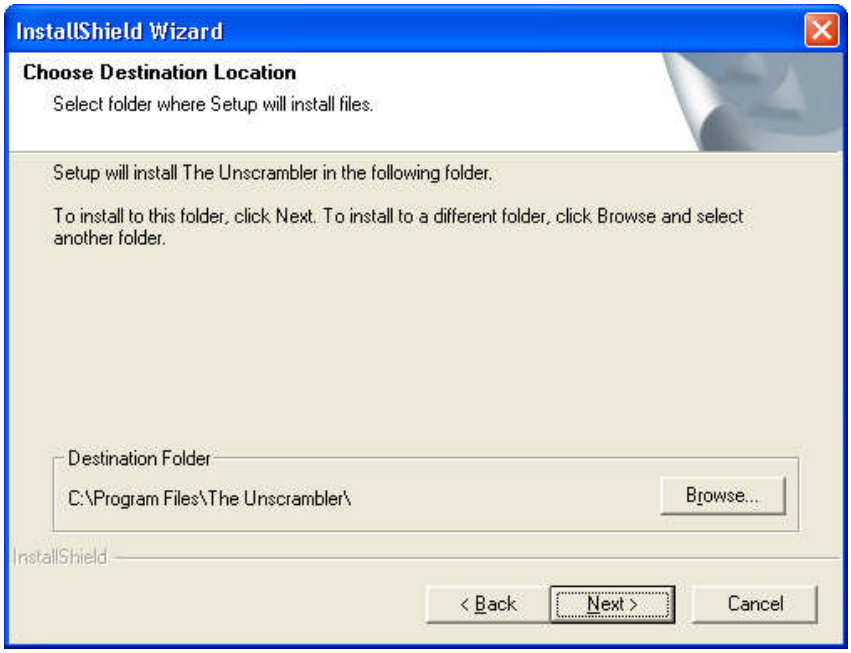
5. The InstallShield Wizard for The Unscrambler is launched


InstallShield Wizard
Welcome to the InstallShield Wizard for The Unscrambler
The InstallShield® Wizard will install The Unscrambler on your computer. To continue, click Next.
< Back
Next >
Cancel

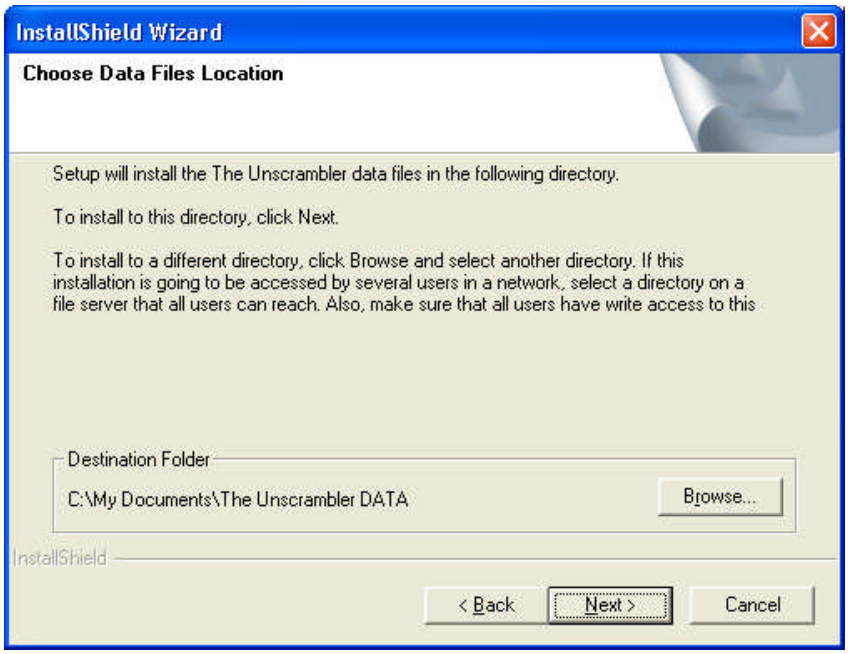
6. Read the licence agreement carefully and click **Yes** to accept the terms of the agreement


InstallShield Wizard
License Agreement
Please read the following license agreement carefully.
Press the PAGE DOWN key to see the rest of the agreement.
IMPORTANT - READ CAREFULLY
The CAMO license agreement is a legal agreement between you (the Licensee) and CAMO PROCESS AS (the Licenser) and the company you bought the software from for the CAMO software product. The software products covered by this agreement is The Unscrambler(R),The Unscrambler(R) Designer, The Unscrambler(R) MVA and The Unscrambler License Server (hereafter referred to as the Program), and includes computer software and associated media and printed materials, and may include on-line or electronic documentation. By installing, copying, or otherwise using the Program, you agree to be bounds by the terms in this license agreement. If you do not agree to the terms in this license agreement, promptly return the unused software to the place from which you
Do you accept all the terms of the preceding License Agreement? If you choose No, the setup will close. To install The Unscrambler, you must accept this agreement.
InstallShield
< Back
Yes
No

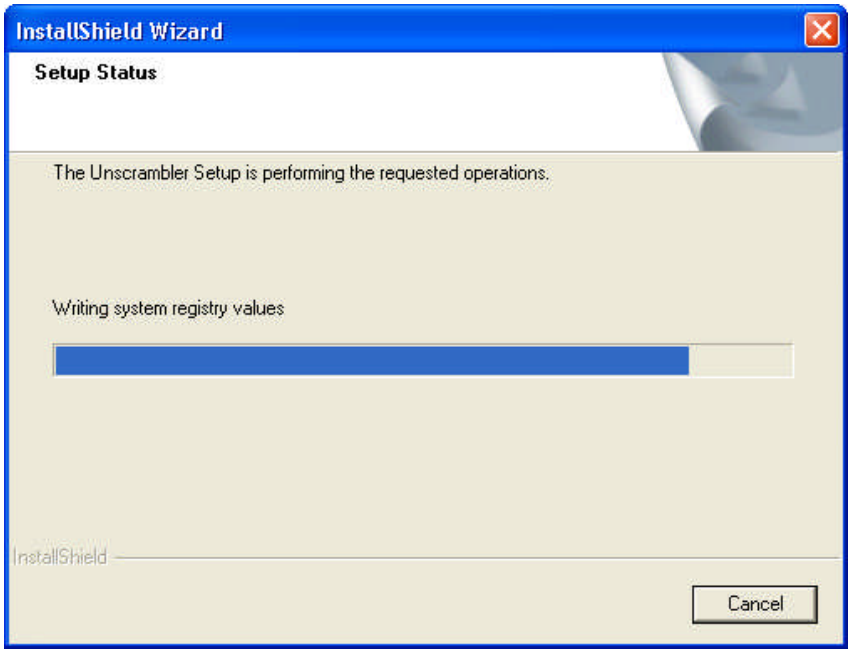
7. Select a destination folder for the The Unscrambler Program files


InstallShield Wizard
Choose Destination Location
Select folder where Setup will install files.
Setup will install The Unscrambler in the following folder.
To install to this folder, click Next. To install to a different folder, click Browse and select another folder.
Destination Folder
C:\Program Files\The Unscrambler\
Browse...
InstallShield
< Back
Next >
Cancel

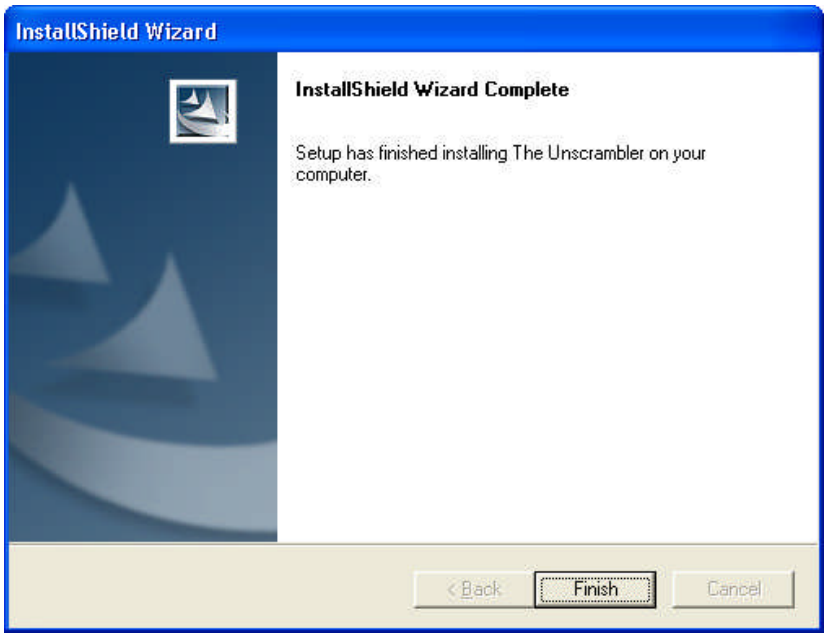
8. Select a destination folder for the The Unscrambler DATA files


InstallShield Wizard
Choose Data Files Location
Setup will install the The Unscrambler data files in the following directory.
To install to this directory, click Next.
To install to a different directory, click Browse and select another directory. If this installation is going to be accessed by several users in a network, select a directory on a file server that all users can reach. Also, make sure that all users have write access to this
Destination Folder
C:\My Documents\The Unscrambler DATA
Browse...
InstallShield
< Back
Next >
Cancel

9. The program is being installed

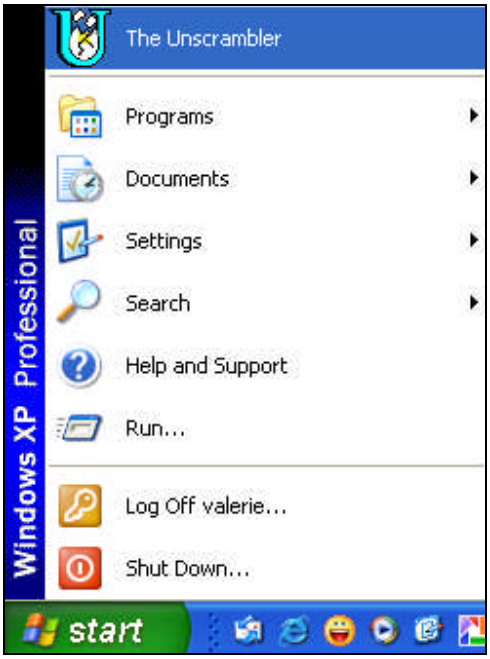


10. When the setup is complete, click **Finish**

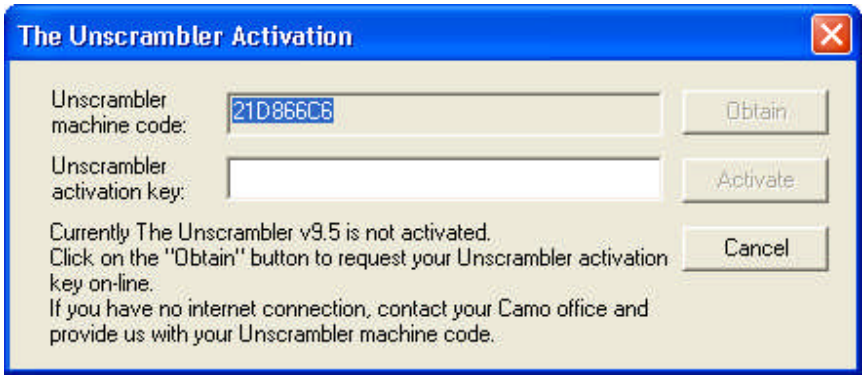


Requesting an Unscrambler Activation Key

11. Start The Unscrambler from the **Start** menu



12. **The Unscrambler Activation** dialog opens.


The Unscrambler Activation
Unscrambler machine code:
21D866C6
Obtain
Unscrambler activation key:
Activate
Currently The Unscrambler v9.5 is not activated.
Click on the "Obtain" button to request your Unscrambler activation key on-line.
If you have no internet connection, contact your Camo office and provide us with your Unscrambler machine code.
Cancel

If you have Internet access…

Click the Obtain button to request your **Unscrambler activation key** online. You will be brought to the activation key request form on Camo's website. When you submit your request, your Unscrambler activation key will be automatically sent to your e-mail ID.

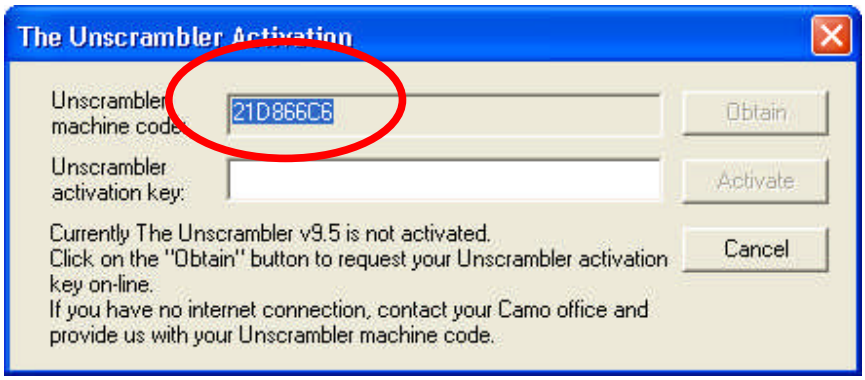
Note!

Your e-mail ID is the means of identifying you as a registered user. Make sure to type in the same e-mail address in the form as the one you registered as an Unscrambler licensee to receive a permanent activation key.

If you are not a registered Unscrambler licensee, a 30-day activation key will be sent to your e-mail ID.

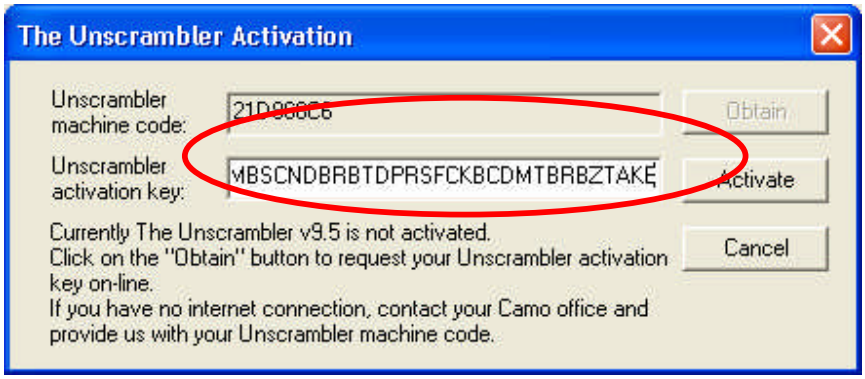
If you do not have Internet access…

Contact Camo and give your Camo consultant the **Unscrambler machine code** that is displayed on screen. Your consultant will provide you with an activation key in accordance to your license.

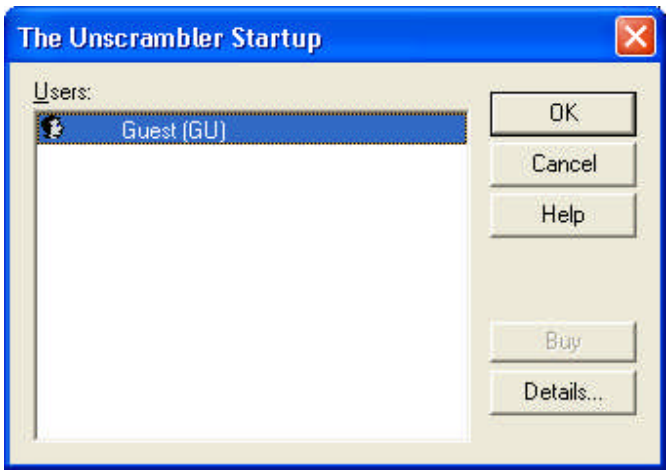

The Unscrambler Activation
Unscrambler machine code:
21D866C6
Obtain
Unscrambler activation key:
Activate
Currently The Unscrambler v9.5 is not activated.
Click on the "Obtain" button to request your Unscrambler activation key on-line.
If you have no internet connection, contact your Camo office and provide us with your Unscrambler machine code.
Cancel

Activating The Unscrambler

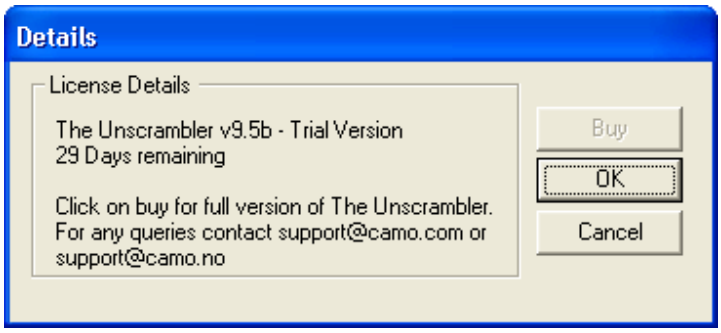
13. Type in your Unscrambler activation key into the relevant field of **The Unscrambler Activation** dialog, then click the Activate button.


The Unscrambler Activation
Unscrambler machine code:
Obtain
Unscrambler activation key:
MBSCNDBRBTDPRSFCKBCDMTBRBZTAKE
Activate
Currently The Unscrambler v9.5 is not activated.
Click on the "Obtain" button to request your Unscrambler activation key on-line.
If you have no internet connection, contact your Camo office and provide us with your Unscrambler machine code.
Cancel

14. The Unscrambler Startup dialog will appear.



You may click the Details… button to check the details of your license.



Defining User Name and Password

User name and password are defined by logging in as supervisor in **The Unscrambler Startup** dialog.

Lookup chapter System Configuration in Practice for detailed instructions.

Network Installation (Multiple-User Licenses)

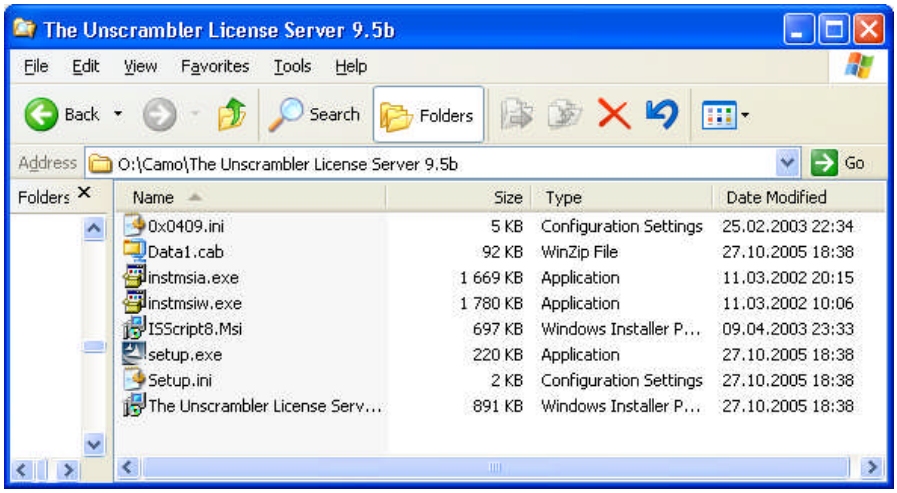
Installing The Unscrambler on a network is a straightforward procedure in eight steps:

1. Download of The Unscrambler License Server
2. Installation of The Unscrambler License Server
3. Request of an Unscrambler License Server Activation Key
4. Activation of The Unscrambler License Server
5. Definition of user names and passwords
6. Configuration Settings
7. Download of The Unscrambler Client
8. Installation of The Unscrambler Client

A detailed description of each of these steps is given below.

Downloading The Unscrambler License Server

1. Download The Unscrambler License Server from www.camo.com and save it into a Temp folder on your server.
2. Extract the file. A folder **The Unscrambler License Server** is created.
3. Double-click on file **setup.exe** to start the installation.

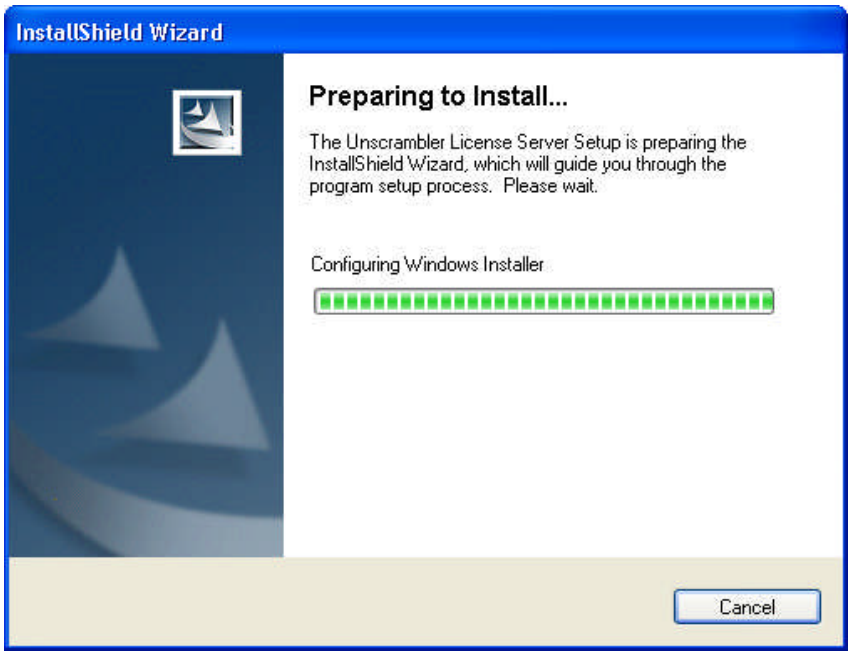

The Unscrambler License Server 9.5b
File Edit View Favorites Tools Help
Back Search Folders
Address O:\Camo\The Unscrambler License Server 9.5b
Go
Folders
Name Size Type Date Modified
0x0409.ini 5 KB Configuration Settings 25.02.2003 22:34
Data1.cab 92 KB WinZip File 27.10.2005 18:38
instmsia.exe 1 669 KB Application 11.03.2002 20:15
instmsiw.exe 1 780 KB Application 11.03.2002 10:06
ISScript8.Msi 697 KB Windows Installer P... 09.04.2003 23:33
setup.exe 220 KB Application 27.10.2005 18:38
Setup.ini 2 KB Configuration Settings 27.10.2005 18:38
The Unscrambler License Serv... 891 KB Windows Installer P... 27.10.2005 18:38

Installing The Unscrambler License Server

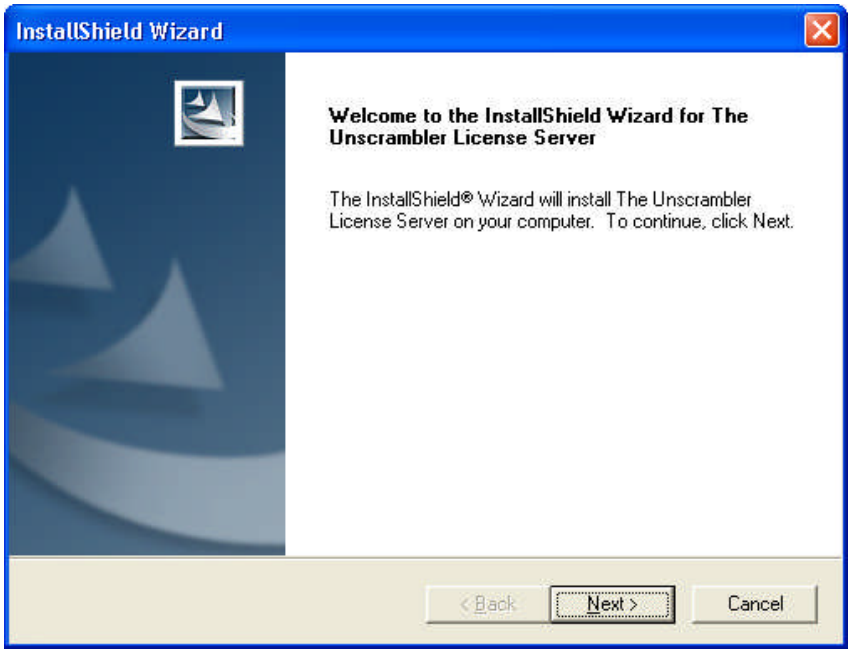
If you have received The Unscrambler License Server installer on CD-ROM, simply place the CD in your CD player.

If you have downloaded The Unscrambler License Server from Camo's website, double-click on file **setup.exe** to start the installation.

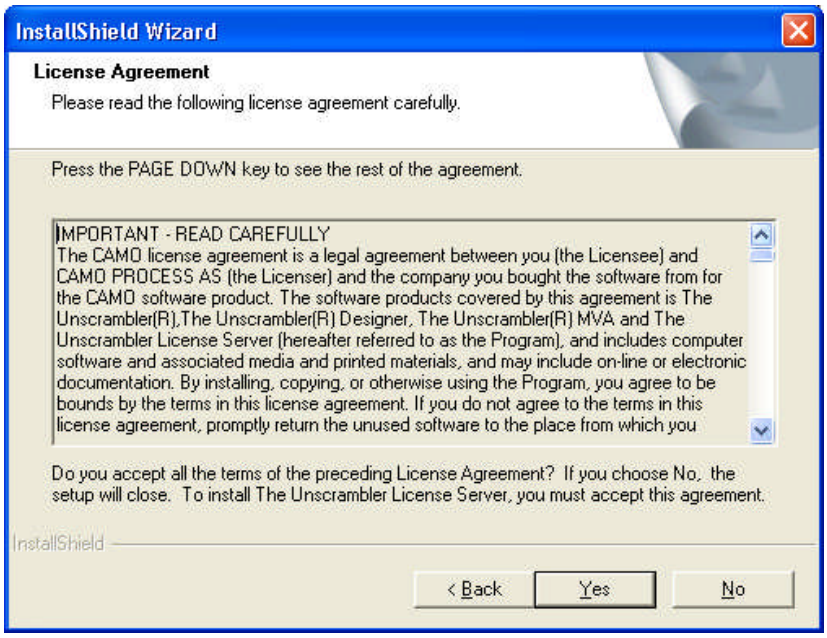
4. An **InstallShield Wizard** dialog opens


InstallShield Wizard
Preparing to Install...
The Unscrambler License Server Setup is preparing the InstallShield Wizard, which will guide you through the program setup process. Please wait.
Configuring Windows Installer
Cancel

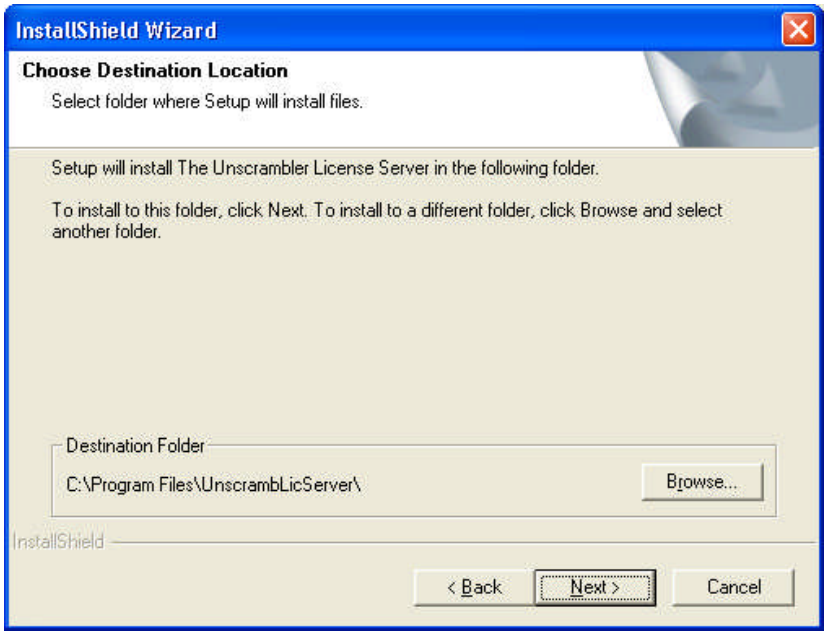
5. The InstallShield Wizard for The Unscrambler License Server is launched


InstallShield Wizard
Welcome to the InstallShield Wizard for The Unscrambler License Server
The InstallShield® Wizard will install The Unscrambler License Server on your computer. To continue, click Next.
< Back
Next >
Cancel

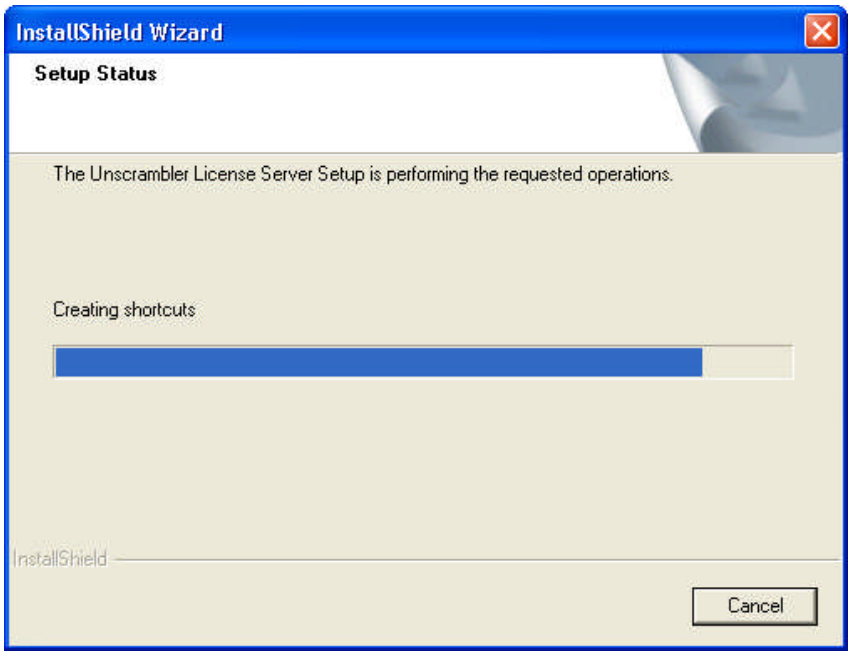
6. Read the licence agreement carefully and click **Yes** to accept the terms of the agreement


InstallShield Wizard
License Agreement
Please read the following license agreement carefully.
Press the PAGE DOWN key to see the rest of the agreement.
IMPORTANT - READ CAREFULLY
The CAMO license agreement is a legal agreement between you (the Licensee) and CAMO PROCESS AS (the Licenser) and the company you bought the software from for the CAMO software product. The software products covered by this agreement is The Unscrambler(R),The Unscrambler(R) Designer, The Unscrambler(R) MVA and The Unscrambler License Server (hereafter referred to as the Program), and includes computer software and associated media and printed materials, and may include on-line or electronic documentation. By installing, copying, or otherwise using the Program, you agree to be bounds by the terms in this license agreement. If you do not agree to the terms in this license agreement, promptly return the unused software to the place from which you
Do you accept all the terms of the preceding License Agreement? If you choose No, the setup will close. To install The Unscrambler License Server, you must accept this agreement.
InstallShield
< Back
Yes
No

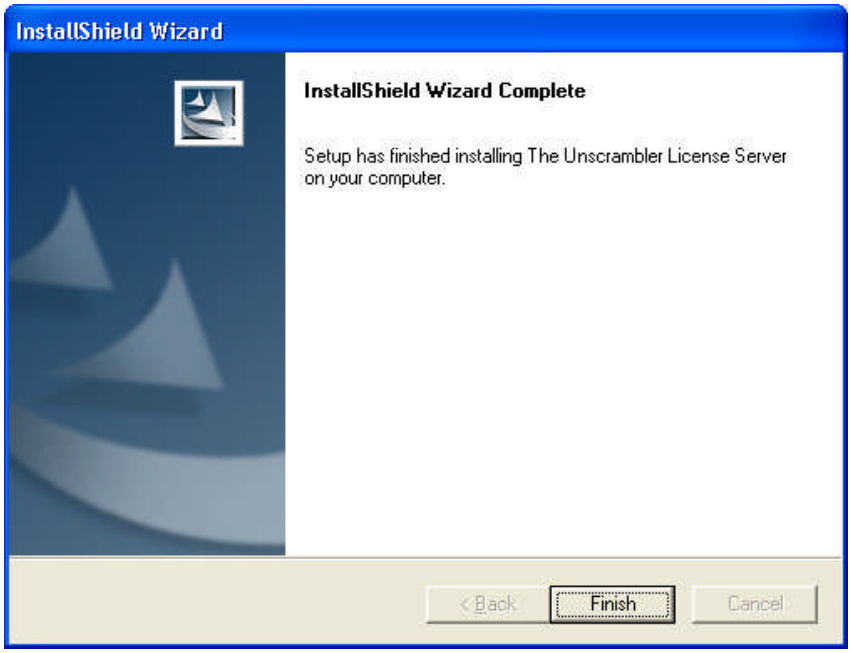
7. Select a destination folder for The Unscrambler License Server


InstallShield Wizard
Choose Destination Location
Select folder where Setup will install files.
Setup will install The Unscrambler License Server in the following folder.
To install to this folder, click Next. To install to a different folder, click Browse and select another folder.
Destination Folder
C:\Program Files\UnscrambLicServer\
Browse...
InstallShield
< Back
Next >
Cancel

8. The program is being installed

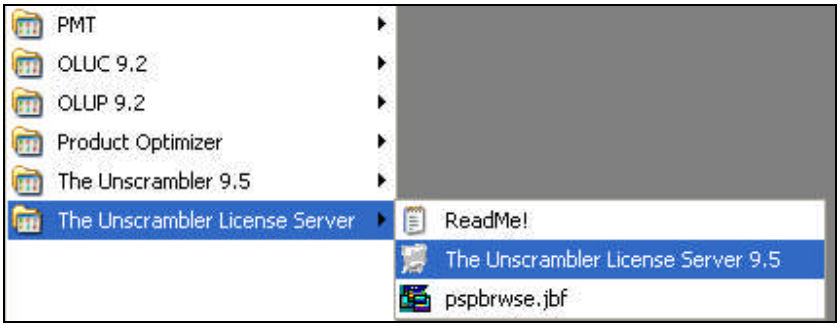


9. When the setup is complete, click **Finish**

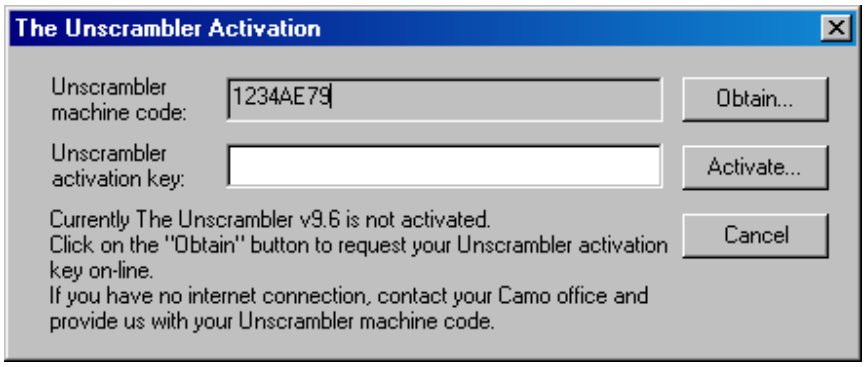


Requesting an Unscrambler License Server Activation Key

10. Start The Unscrambler License Server from menu **Start - Programs - The Unscrambler License Server**



11. **The Unscrambler License Server Activation** dialog opens.


The Unscrambler Activation
Unscrambler machine code:
1234AE79
Obtain...
Unscrambler activation key:
Activate...
Currently The Unscrambler v9.6 is not activated.
Click on the "Obtain" button to request your Unscrambler activation key on-line.
If you have no internet connection, contact your Camo office and provide us with your Unscrambler machine code.
Cancel

If you have Internet access…

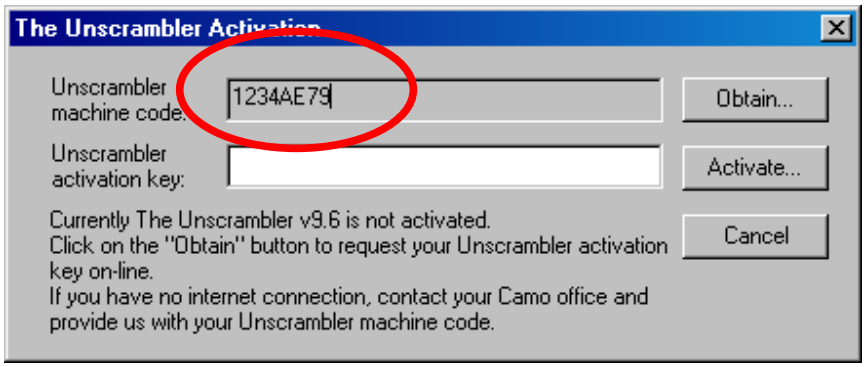
Click the Obtain button to request your **Unscrambler License Server activation key** online. You will be brought to the activation key request form on Camo's website. When you submit your request, your Unscrambler activation key will be automatically sent to your e-mail ID.

Note!

Your e-mail ID is the means of identifying you as a registered licensee. Make sure to type in the same e-mail address in the form as the one you registered as an Unscrambler licensee to receive a permanent activation key.

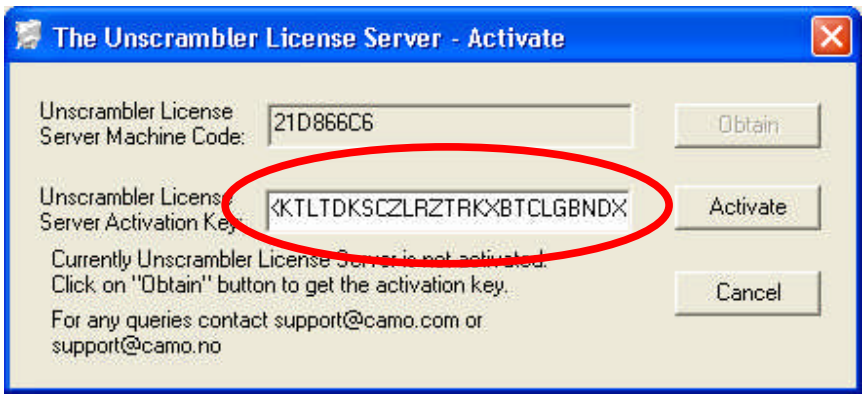
If you do not have Internet access…

Contact Camo and give your Camo consultant the **Unscrambler License Server machine code** that is displayed on screen. Your consultant will provide you with an activation key in accordance to your network license.


The Unscrambler Activation
Unscrambler machine code:
1234AE79
Obtain...
Unscrambler activation key:
Activate...
Currently The Unscrambler v9.6 is not activated.
Click on the "Obtain" button to request your Unscrambler activation key on-line.
If you have no internet connection, contact your Camo office and provide us with your Unscrambler machine code.
Cancel

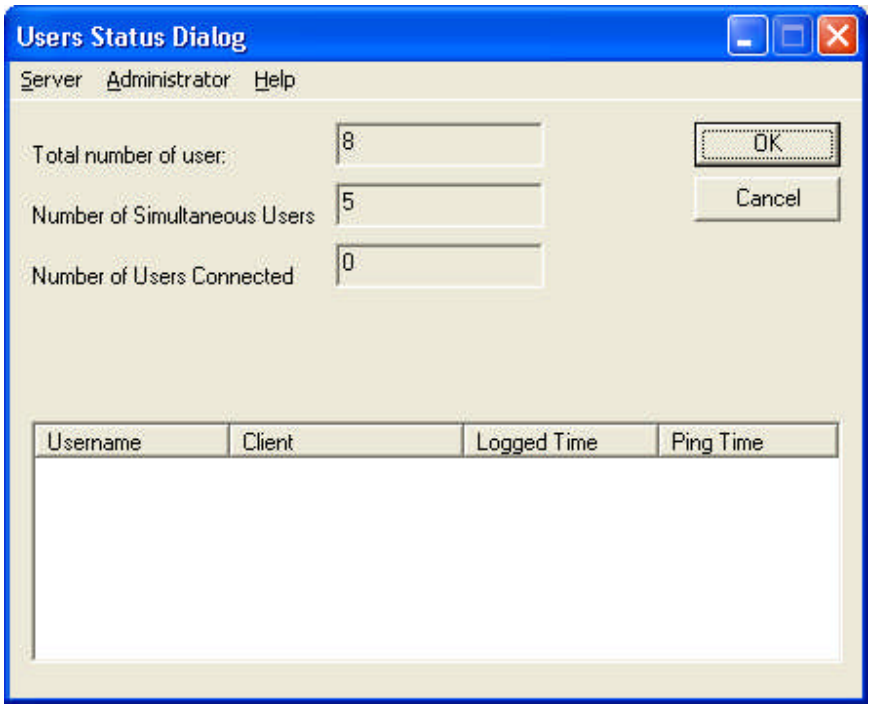
Activating The Unscrambler License Server

12. Type in your Unscrambler License Server activation key into the relevant field of **The Unscrambler Activation** dialog, then click the Activate button.


The Unscrambler License Server - Activate
Unscrambler License Server Machine Code:
21D866C6
Obtain
Unscrambler License Server Activation Key:
KTLTDKSCZLRZTRKXBTCLGBNDX
Activate
Currently Unscrambler License Server is not activated.
Click on "Obtain" button to get the activation key.
For any queries contact support@camo.com or support@camo.no
Cancel

13. A message confirms that the activation was successful.

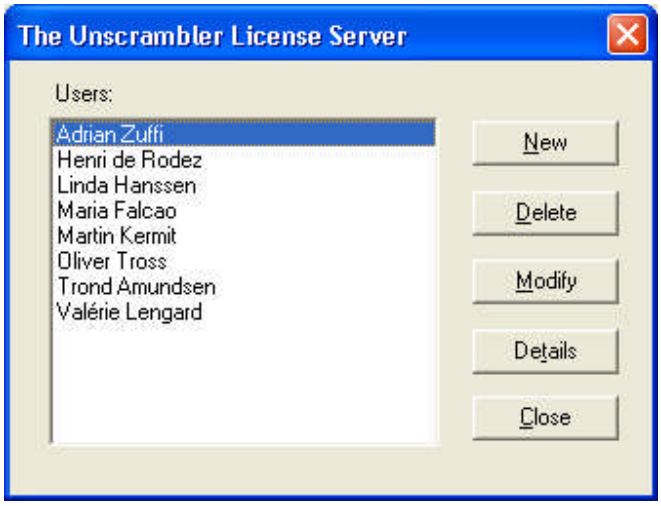
14. The **Users Status Dialog** will appear.



The dialog box indicates the total number of users and the number of simultaneous users authorized by your network license.

Defining User Names and Passwords

Use menu **Administrator - Users** in the **Users Status Dialog** to access the dialog box for user names and password definition. Passwords must be between 6 and 15 characters in length and must be a combination of numbers and letters.

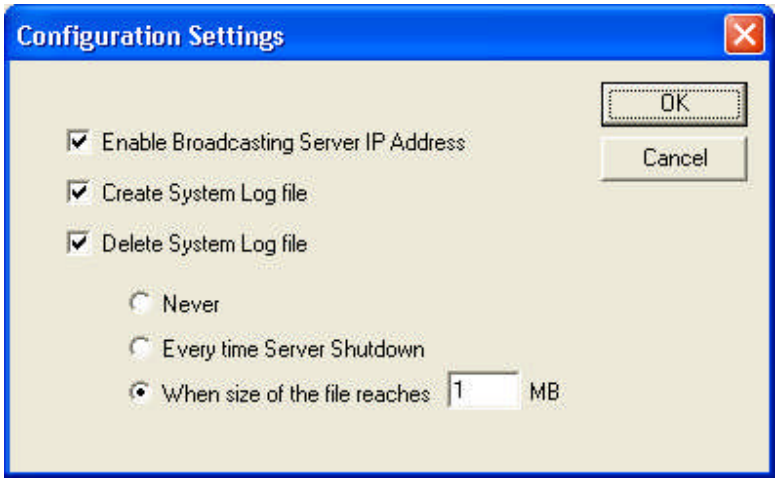


Note!

In the **New User** dialog box, it is important *not* to check the Can empty log option if your company is submitted to traceability regulations and 21 CFR Part 11 FDA guidelines for electronic recording. This option would allow the user to delete the Unscrambler's log trail of data files changes and model files generation.

Configuring Settings

Use menu **Administrator - Options** in the **Users Status Dialog** to open the **Configuration Settings** dialog, where you may configure the system log file.



Downloading The Unscrambler Client

15. Download The Unscrambler Client installer from www.camo.com and save it in a shared location on your network.
16. Extract the files. A folder **The Unscrambler Client** is created.
17. From each client machine, double-click on file **setup.exe** to start the installation.

Installing The Unscrambler Client

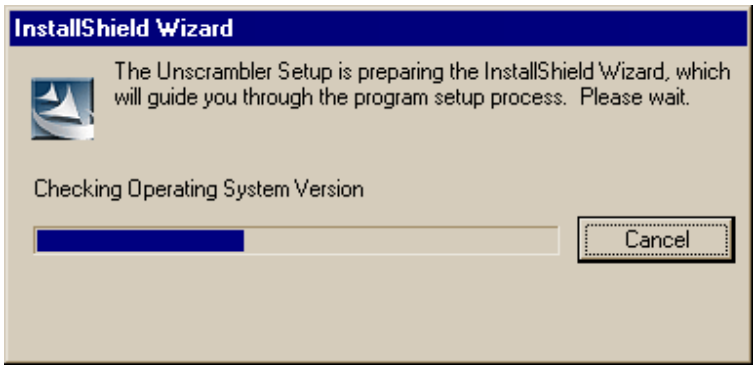
If you are upgrading to a new version, it is recommended to uninstall your previous Unscrambler installation prior to installing the new one.

Un-installing your former Unscrambler version will remove the program files only; all your Unscrambler data files and model files will be preserved.

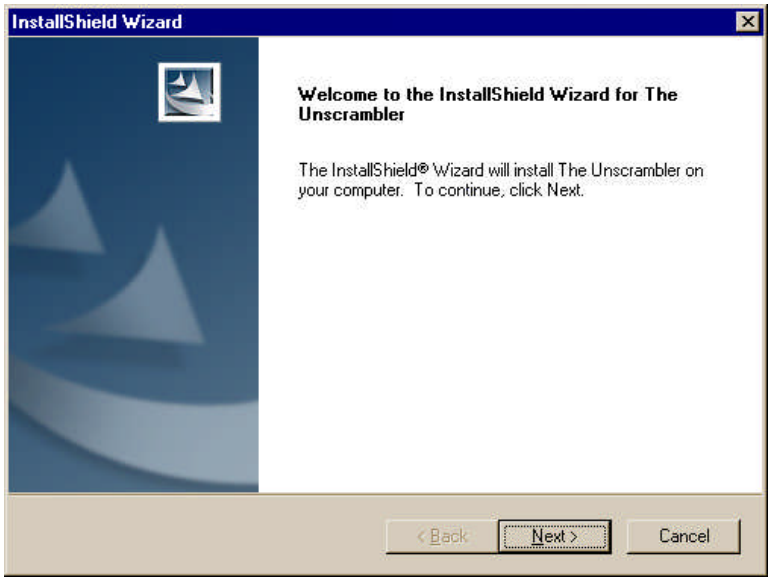
18. If you have downloaded The Unscrambler from Camo's website, double-click on file **setup.exe** file found in folder **The Unscrambler Client** to start the installation.

    If you have received The Unscrambler installer on CD-ROM, place the CD in your CD player.

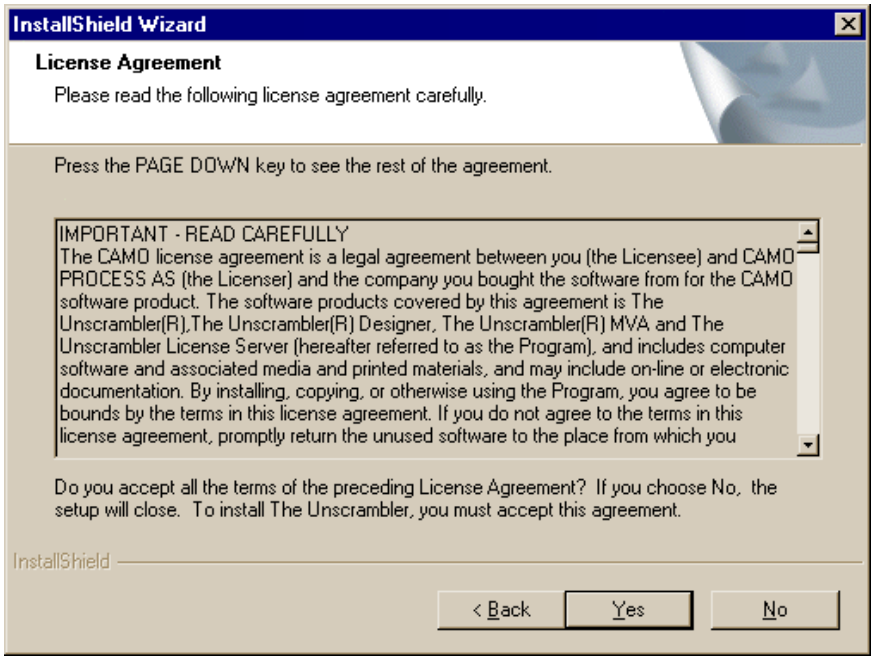
19. An **InstallShield Wizard** dialog opens


InstallShield Wizard
The Unscrambler Setup is preparing the InstallShield Wizard, which will guide you through the program setup process. Please wait.
Checking Operating System Version
Cancel

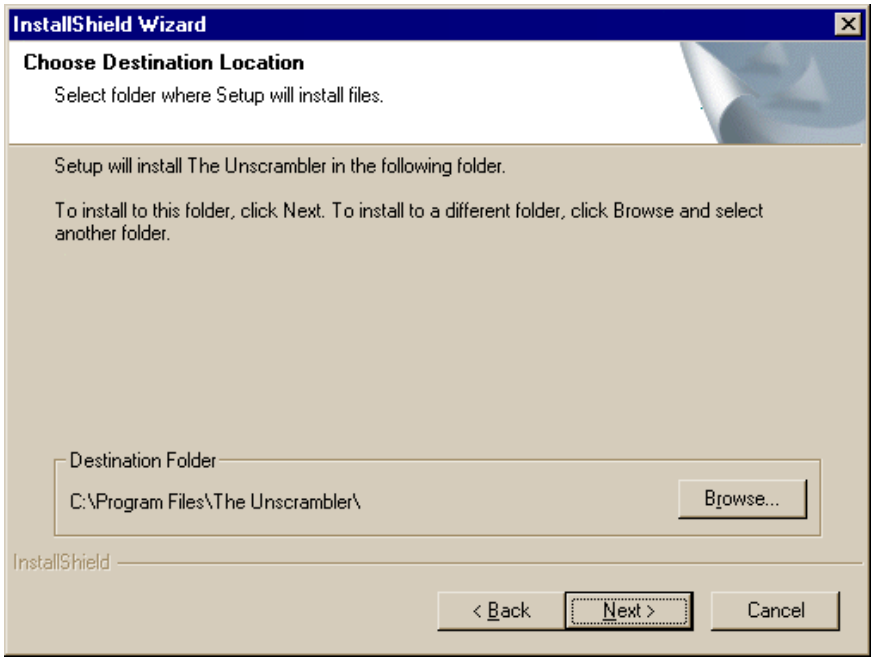
20. The InstallShield Wizard for The Unscrambler is launched


InstallShield Wizard
Welcome to the InstallShield Wizard for The Unscrambler
The InstallShield® Wizard will install The Unscrambler on your computer. To continue, click Next.
< Back
Next >
Cancel

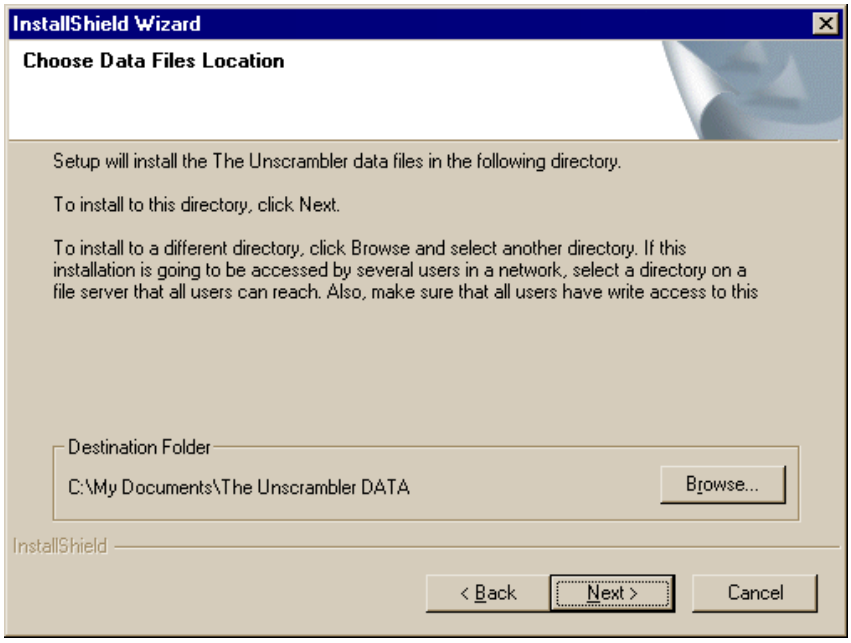
21. Read the licence agreement carefully and click **Yes** to accept the terms of the agreement


InstallShield Wizard
License Agreement
Please read the following license agreement carefully.
Press the PAGE DOWN key to see the rest of the agreement.
IMPORTANT - READ CAREFULLY
The CAMO license agreement is a legal agreement between you (the Licensee) and CAMO PROCESS AS (the Licenser) and the company you bought the software from for the CAMO software product. The software products covered by this agreement is The Unscrambler(R),The Unscrambler(R) Designer, The Unscrambler(R) MVA and The Unscrambler License Server (hereafter referred to as the Program), and includes computer software and associated media and printed materials, and may include on-line or electronic documentation. By installing, copying, or otherwise using the Program, you agree to be bounds by the terms in this license agreement. If you do not agree to the terms in this license agreement, promptly return the unused software to the place from which you
Do you accept all the terms of the preceding License Agreement? If you choose No, the setup will close. To install The Unscrambler, you must accept this agreement.
InstallShield
< Back
Yes
No

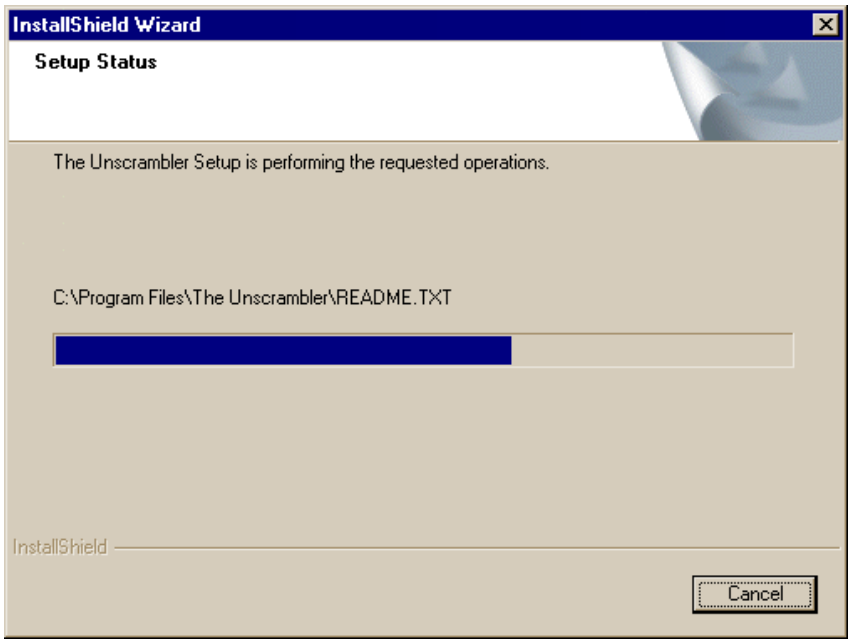
22. Select a destination folder for the The Unscrambler Program files


InstallShield Wizard
Choose Destination Location
Select folder where Setup will install files.
Setup will install The Unscrambler in the following folder.
To install to this folder, click Next. To install to a different folder, click Browse and select another folder.
Destination Folder
C:\Program Files\The Unscrambler\
Browse...
InstallShield
< Back
Next >
Cancel

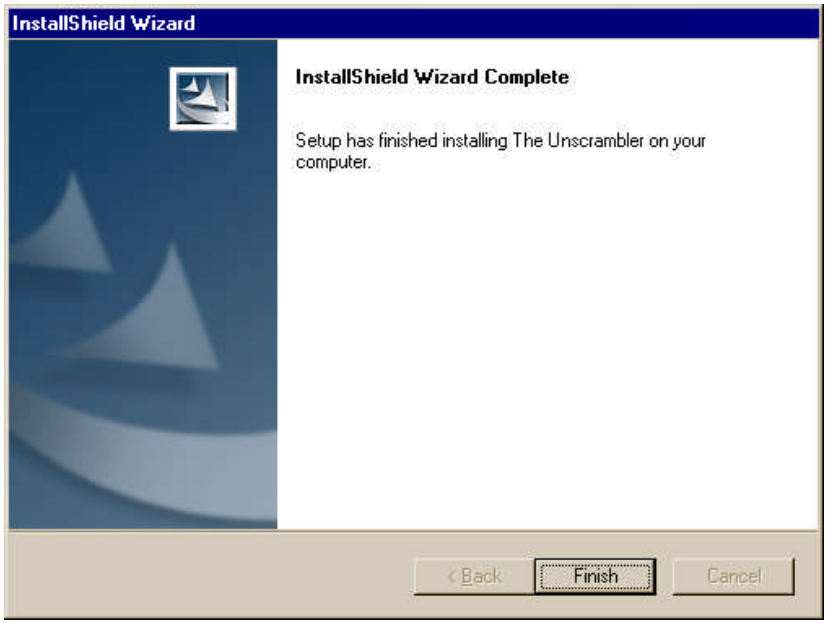
23. Select a destination folder for the The Unscrambler DATA files


InstallShield Wizard
Choose Data Files Location
Setup will install the The Unscrambler data files in the following directory.
To install to this directory, click Next.
To install to a different directory, click Browse and select another directory. If this installation is going to be accessed by several users in a network, select a directory on a file server that all users can reach. Also, make sure that all users have write access to this
Destination Folder
C:\My Documents\The Unscrambler DATA
Browse...
InstallShield
< Back
Next >
Cancel

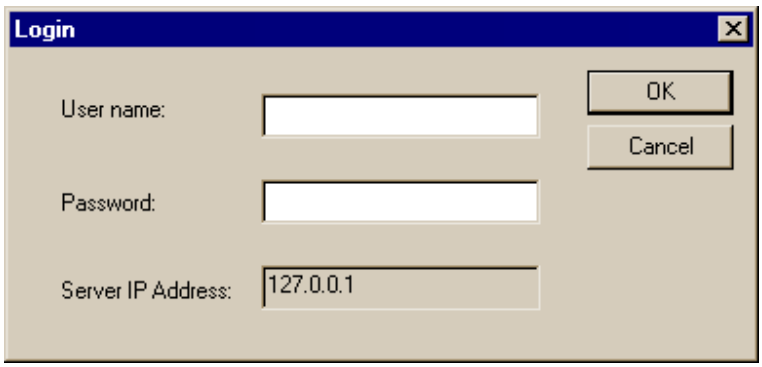
24. The program is being installed



25. When the setup is complete, click **Finish**



26. Start The Unscrambler Client from the **Start** menu. A login dialog will appear. Type in your user name and password to start the application.



Troubleshooting under Installation

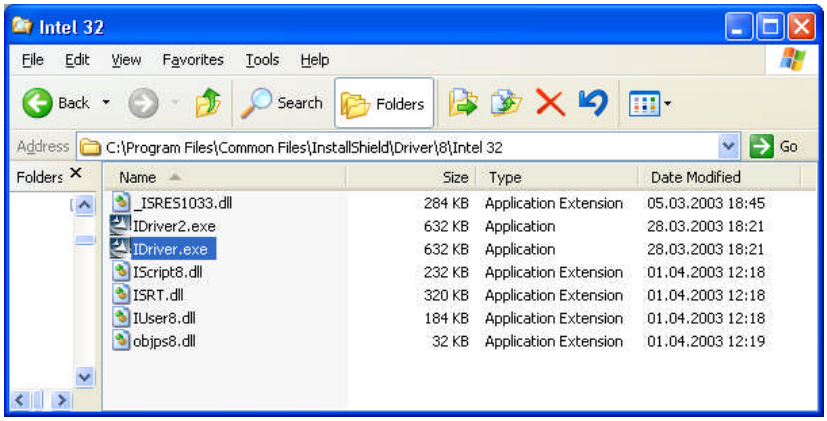
Symptom 1: InstallShield Error Message

When running the **setup.exe** file of The Unscrambler or of The Unscrambler License Server installer, the following message appears:

To solve this problem, double-click on file **IDriver.exe** located in path:

C:\Program Files\Common Files\InstallShield\Driver\8\Intel 32

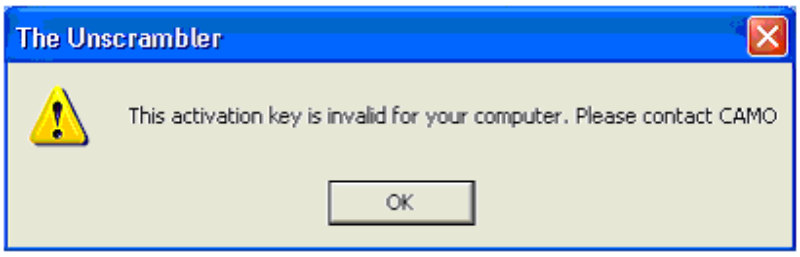
or similar location.


Intel 32
File Edit View Favorites Tools Help
Back Search Folders
Address C:\Program Files\Common Files\InstallShield\Driver\8\Intel 32
Go
Folders
Name Size Type Date Modified
_ISRES1033.dll 284 KB Application Extension 05.03.2003 18:45
IDriver2.exe 632 KB Application 28.03.2003 18:21
IDriver.exe 632 KB Application 28.03.2003 18:21
IScript8.dll 232 KB Application Extension 01.04.2003 12:18
ISRT.dll 320 KB Application Extension 01.04.2003 12:18
IUser8.dll 184 KB Application Extension 01.04.2003 12:18
objps8.dll 32 KB Application Extension 01.04.2003 12:19

Then double-click on the **setup.exe** again to execute it.

Symptom 2: Invalid Activation Key

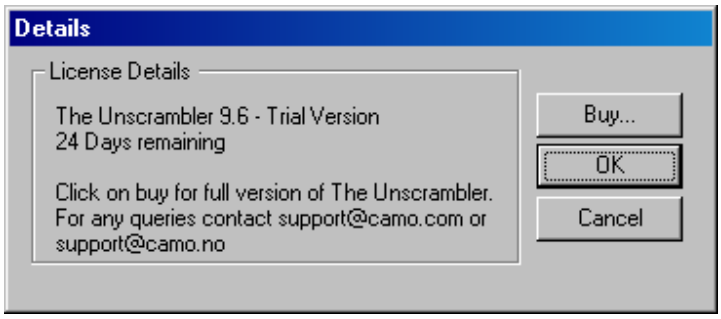
When clicking the Activate button in **The Unscrambler Activation** dialog, the following message might appear:



This message will occur if the Unscrambler License Server activation key you have input is not valid for your machine. Provide Camo with your machine code to receive the appropriate activation key for your machine (see Requesting an Unscrambler Activation Key above).

Symptom 3: Incorrect License Details in Standalone Installation

The license details information of your Unscrambler Standalone installation doesn't correspond to the type of license you have purchased from Camo. For example, the license appears to be a 30-day license instead of a permanent license.



This situation may occur if when requesting an activation key, you have not utilised your registered licensee e-mail ID, but a different e-mail ID.

Login as supervisor (see section System Configuration in Practice) and click on menu **Help - Change License…** to request a new activation key. Upon submitting your new request, make sure to use your registered licensee e-mail ID.

If you do not remember what your registered licensee e-mail ID is, contact Camo and your consultant will either give you the information, or update your registered licensee e-mail ID to a new one in Camo's licensing database.

Symptom 4: The Unscrambler Previous Version was not Upgraded to the New Version

If under starting up The Unscrambler the old version number is indicated instead of the new version number, it indicates that the upgrade has not performed properly. The version number of the application is also accessible in menu **Help - About…**

Close the Unscrambler application, un-install your previous Unscrambler installation, then run the new installation again.

Un-installing your former Unscrambler version will remove the program files only; all your Unscrambler data files and model files will be preserved.

Symptom 5: No Activation Key is Required in Standalone Installation

If under starting up The Unscrambler in a standalone installation no activation key is required, it indicates that the upgrade has not performed properly.

Close the Unscrambler application, un-install your previous Unscrambler installation, then run the new installation again.

Un-installing your former Unscrambler version will remove the program files only; all your Unscrambler data files and model files will be preserved.

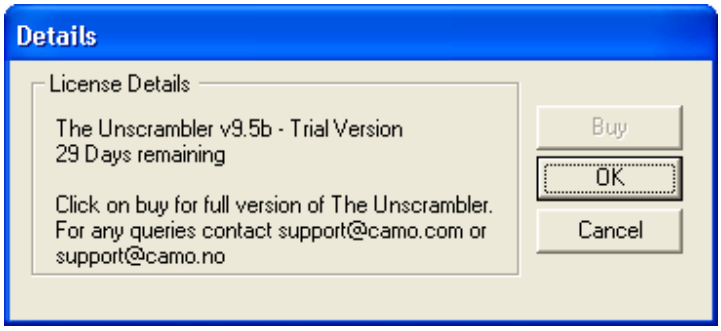
Upgrade from Trial Installation to Permanent License

Even if you are not a registered licensee, you may download and install a trial installation of The Unscrambler Standalone.

Once you have tested the program, you may find out that you want to purchase it.

Upon starting The Unscrambler, click Details in the **Startup Dialog** to display the **Details dialog** showing your license details.

Dialog: Details



Contact Camo to place your order.

Once you are registered as Unscrambler licensee in Camo's customer database, you may proceed in upgrading to a permanent license; this is done very simply with a new activation key.

Log in as supervisor (see section System Configuration in Practice) and click on menu **Help - Change License…** to request a new activation key. Upon submitting your new request, make sure to use your registered licensee e-mail ID.

System Configuration

Once The Unscrambler is installed, the system supervisor may define new users and specify general options.

Supervisor Responsibilities

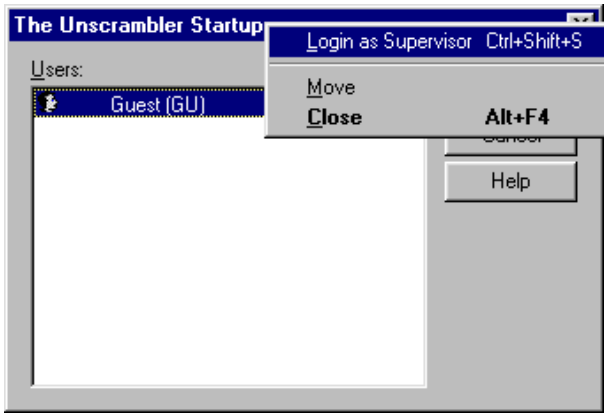
The Unscrambler requires that one person is appointed as ***supervisor*** (system manager). The supervisor's main task is to maintain the user accounts. In a single-user installation of The Unscrambler, you are your own supervisor.

The supervisor must log in after installation and define the users who are allowed access to Unscrambler before they can begin to work with the program. In a single-user installation, this simply means that you have to log in as Supervisor in order to modify the default user "Guest" and give it a name of your choice (usually, your own name).

System Configuration in Practice

Start The Unscrambler and log in as Supervisor by right-clicking on the caption bar in the **Startup dialog** or pressing <Ctrl>+<Shift>+<S> (see the figure below).

Dialog: The Unscrambler Startup



This triggers the **Login dialog** where you may log in as Supervisor by typing in the correct password. The default supervisor password at delivery is SYSOP.

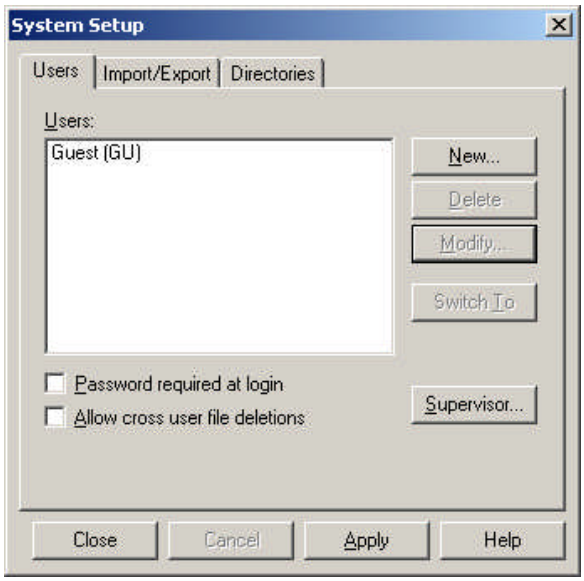
User accounts are maintained from **File - System Setup**. The **System Setup** dialog consists of 3 sheets:

- Users
- Import/Export
- Directories

System Setup Dialog: Users Sheet

As supervisor, you can add a new user, delete an existing user or modify user properties.

Dialog: System Setup, Users sheet



- New users are added by pressing New. For a single-user license, you have to delete the existing user before you can create a new one (or alternately use Modify on the existing user).
- An existing user can be deleted by pressing Delete.
- Select a user from the **Users** list and press Modify to change the user's name or password.
- Select a user from the list and press Switch To to log in as that user.
- Press Supervisor to change the Supervisor's password.

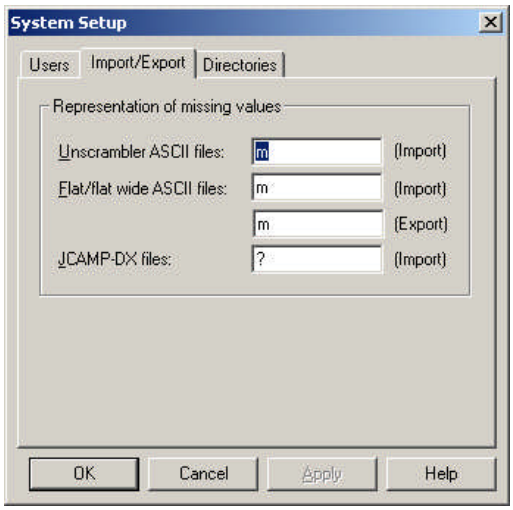
At the bottom of the sheet, the Password required at login tick box allows you to activate the passwords of users other than Supervisor (which is always active).

Tick Allow cross-user file deletions if you wish to allow all users to delete files that were created by other users.

System Setup Dialog: Import/Export Sheet

The supervisor can define how missing values should be handled by default when users import or export data.

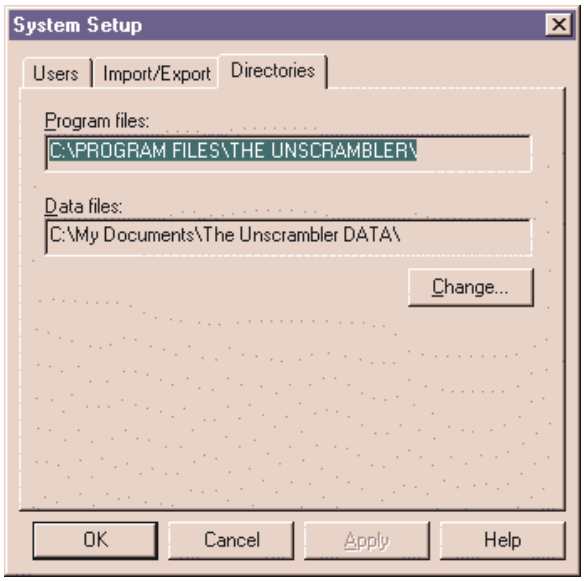
Dialog: System Setup, Import/Export sheet



System Setup Dialog: Directories Sheet

The supervisor can move the data directory to a new location by pressing Change on the **Directories** sheet (see the figure below).

Dialog: System Setup, Directories sheet



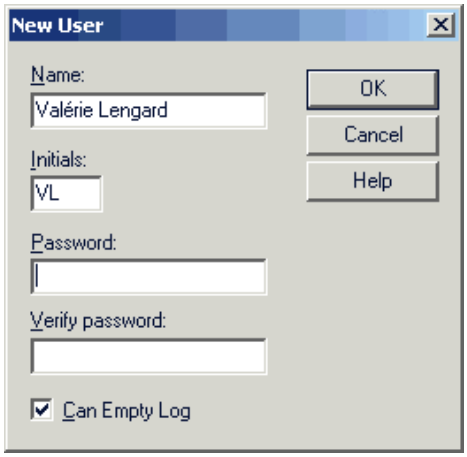
Note that the data files are ***copied*** to the new location, not physically moved. This ensures that a backup exists if the location change fails for some reason. The previous data directory can be removed manually if desired.

New User / Modify User / Modify Supervisor Dialog

The dialogs for specifying a new user, modifying an existing user and modifying the Supervisor are alike. They are accessed by clicking New… (resp. Modify… or Supervisor…) from the **Users** sheet of the **System Setup** dialog when you are logged in as Supervisor.

In this dialog, the supervisor specifies the user's name, initials and personal password.

Dialog: New User



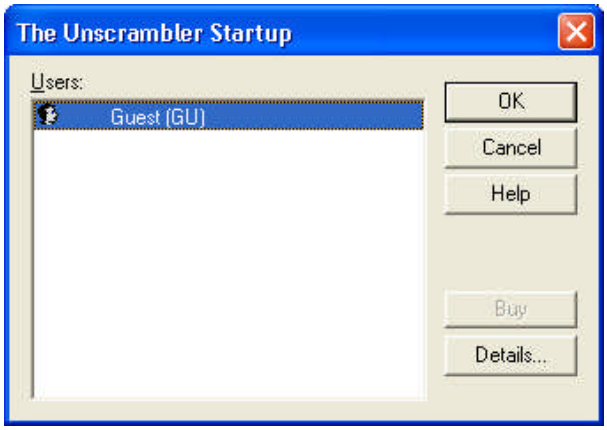
The name and initials defined in this dialog will be traceable in any data or model files that the user creates in The Unscrambler.

The option Can Empty Log (which is active by default) may be ticked off (made inactive) to prevent the user from deleting Log trail information. The Log trail is automatically recorded and updated each time a data file is in use.

Startup Dialog

This dialog pops up when you start The Unscrambler, either from the **Start** menu of Windows, by double-clicking on the Unscrambler icon, or by double-clicking on the **Unscramb.exe** file.

Dialog: The Unscrambler Startup

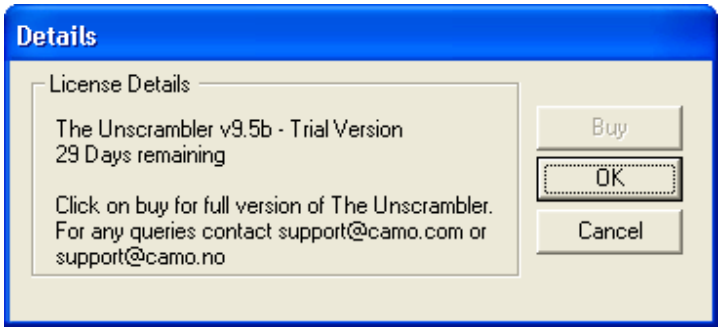


In this dialog, you have to select a user name from the list, then click OK. If the user you have selected requires a password, you enter the **Login** dialog; else the Unscrambler starts right away.

By default, The Unscrambler is delivered with a single user name: Guest (GU). If you wish to add more user names and/or apply changes to an existing user name, you (or your system administrator) will have to log in as Supervisor. See section System Configuration in Practice for more details on how to do this.

You may also click the Details… button to check the details of your license.

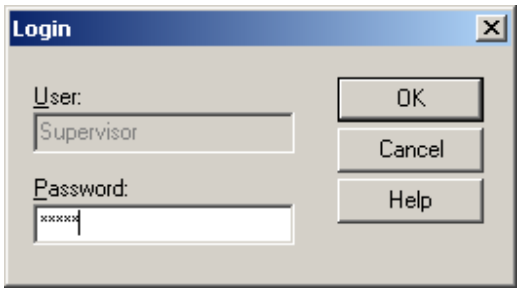
Dialog: Details



Login Dialog

This dialog pops up once you have chosen a user name from the Startup dialog, if the chosen user has a password and the system Supervisor has activated all passwords.

Dialog: Login (here, as Supervisor)



Type in your password and click OK.

To remove the password, you have to log in as supervisor (see System Configuration in Practice).

General User Interface

Beginners, get your marks in The Unscrambler!

The purpose of this chapter is to give you a global introduction to the principles at use in The Unscrambler. In what follows, you will be provided with a short overview of the Unscrambler user interface or workplace.

Working with Windows®

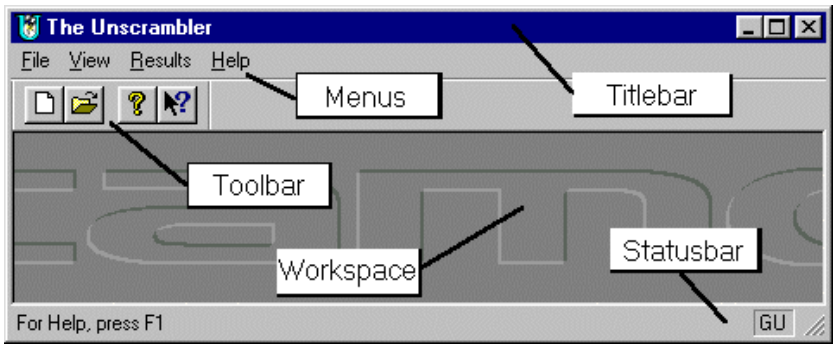
The Unscrambler runs under Windows 95, Windows 98, Windows NT (3.51 or later), Windows 2000 and Windows XP.

We will assume that you are already familiar with the operating system you are using. If not, we recommend that you become fully acquainted with it before starting to work with The Unscrambler. This manual does not explain in detail important points such as the Windows graphical interface, common use of the mouse, etc. Refer to your Windows user guide for more information.

Startup: The Main Window

When you start The Unscrambler, you enter the Main Window, as seen in the figure below.

The Unscrambler main window



The Menu Bar

All operations in The Unscrambler are performed with the help of the menus and options available to you on the Menu bar. The figure above shows the default menus which are enabled when you load The Unscrambler, which all in turn contain several sub-menus and options. When you have an Editor or a Viewer open, more menus will be available. Some sub-menus and options may be invalid in a given context; these are grayed out.

Context Sensitive Menus

The Unscrambler also features so-called context sensitive menus. You access these by clicking the right mouse button while the cursor rests on the area on which you want to perform an operation. The context sensitive menus are a kind of short-cut, as they contain only the options which are valid for the selected area, which will save you the work of having to click your way through all the menus on the Menu bar.

The Toolbar

The Toolbar buttons give you shortcuts to the most frequently used commands. When you let the mouse cursor rest on a toolbar button, an short explanation of its function appears.

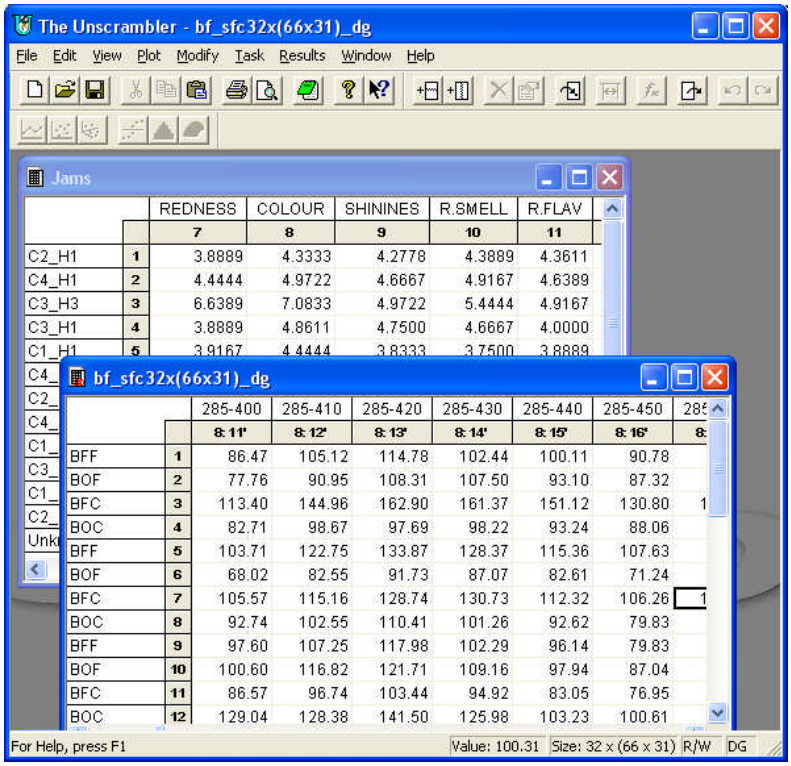
The Status Bar

The Status bar at the bottom of the screen displays concise information. A short explanation of the current menu option is displayed to the left. On the right-hand side, additional information, such as the value of the current cell in the Editor and the size of the data table, is displayed.

Working with Data Tables: The Editor

The Editor, as seen in the figure below, handles data in The Unscrambler. Each time you open or create a data file, its contents will appear in an Editor window. You can open several Editors with different contents at the same time, switching from one to another as you wish. Each time we mention the Editor in this manual and the Help system, we mean a window where data or results are displayed in a tabular form.

The Unscrambler Editor



The Editor: Basic Notions

The Editor consists of a data table made up of rows and columns. The intersection of a column and a row is called a cell; each cell holds a data value. The rows and columns correspond to samples and variables respectively. Samples and variables are identified by a number **and** a name.

The Editor: Active Cell and Cell Selection

At any given time, one cell in an Editor is active. The active cell is marked with a frame. Activate a cell by using the arrow keys to position the cursor or by clicking with the left mouse button on it.

You can also select a range of cells in the Editor, i.e. one or more columns, or one or more rows.

A whole row or column can be selected by clicking with the left mouse button on the sample or variable number (the gray area between the names and the data table itself). Keep the button down and drag the cursor to select more rows or columns. Selecting a new range removes the last range.

To add new samples or variables to an existing selection and to make a range, press the <Ctrl> key while you click on the appropriate samples or variables. The range may be continuous or non-continuous. You can also deselect a sample or variable by pressing the <Ctrl> key while clicking on the object you want to remove from the range, in toggle action. This is only possible with the mouse.

Hold down the <Shift> key while you make the selection if you want to select a continuous block of samples or variables between the last selection and the present selection.

When you make a selection, you always mark either samples or variables, i.e. you either select some variables for all samples or some samples for all variables. You can also mark the whole matrix, but the selection is still sample or variable oriented. You can see whether you are marking samples or variables by looking at the shape of the mouse pointer as you make the selection:

The shape of the mouse pointer when marking samples and variables respectively

Mark Samples:

Mark Variables:

The Editor: Screen Layout

If the data table is larger than the screen, you can scroll the Editor.

Information about the active cell is displayed in The Unscrambler's status bar. Variable names are displayed in black if the variable is continuous and in blue if it is a category variable. Locked cells, e.g. design variables, are grayed out to show that they cannot be edited.

The Editor: Filling Missing Values

If a data table contains some missing values, those may be filled with estimated values that take into account the underlying data structure.

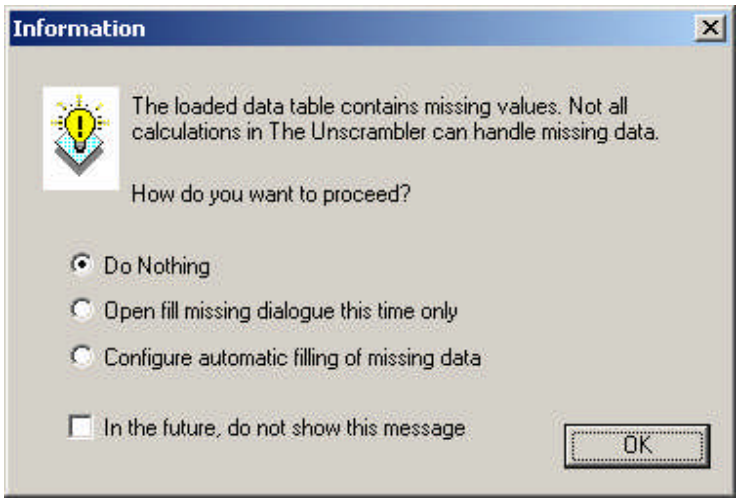
There are two ways of doing this:

- One table at a time: use menu option **Edit - Fill Missing** when your table is displayed in the Editor. This allows you to select the *scope* of the replacement (it need not apply to the whole data table).
- Automatically fill missing values for all data tables: use menu option **File - System Setup** and select the appropriate options in the **Missing Data** sheet. You may select to be notified every time missing values are filled. If so, the following information dialog will appear every time this happens:

Automatic filling of missing values upon opening a data table in the Editor

Note: Unless you have chosen automatic filling of missing values, the **Information** dialog below will appear every time you open a data table containing some missing values in the Editor. You may check a box at the bottom of that dialog to turn it off in the future.

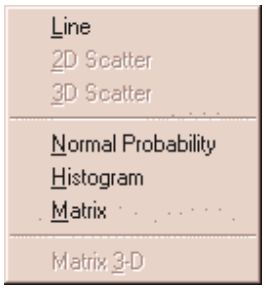
Dialog: Information (upon opening a data table with some missing values)


Information
The loaded data table contains missing values. Not all calculations in The Unscrambler can handle missing data.
How do you want to proceed?
Do Nothing
Open fill missing dialogue this time only
Configure automatic filling of missing data
In the future, do not show this message
OK

Plotting from the Editor

You can easily plot from the Editor: Select the samples or variables you want to look at graphically and select the plot type you want from the **Plot** menu, as seen in the figure below. You can choose between several different plots, depending on how many samples (resp. variables) you have selected. A dialog will appear, in which you select which Variable (resp. Sample) Set to plot. If necessary, you may then click Define to enter the **Set Editor** where new sets can be defined.

Options in the Plot menu when one variable is selected in a 2-D data table



Plotting and Interpreting Results: The Viewer

In the Viewer, data and results are visualized graphically in an interactive manner. Whenever you make a plot, it appears in a Viewer. Every time the ***Viewer*** is mentioned throughout this manual and Help system, we are referring to a window where a plot is displayed.

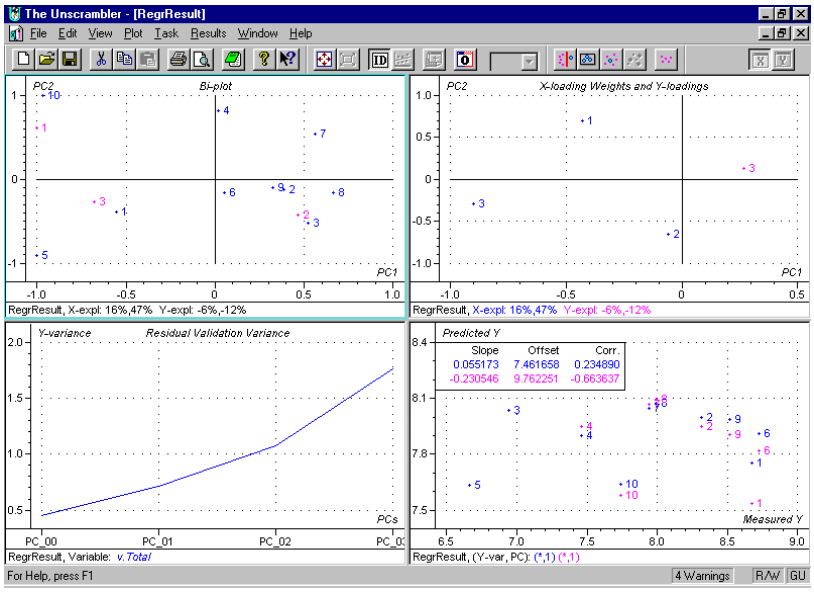
Several Viewers can be open at the same time. In addition, one Viewer can display several plots. This is possible because the Viewer is divided into seven so-called sub-views, organized as shown:

Organization of sub-views

Sub-view	Layout	Sub-view	Layout
1		4	
2		5	
3		6	
		7	

The figure below shows a typical Viewer with sub-views 4–7.

The Unscrambler Viewer



Plotting from the Viewer

Data and results can be plotted in three different ways, of which the last two are done from the Viewer:

- Display a selected part of the data table from the Editor;
- Display data from any data table or result matrix;
- Display predefined result plots from an analysis.

Display Data from a Table or Result Matrix

You do this by selecting **Results - General View**. An empty Viewer appears, giving you access to all data and result files from the **Plot** menu.

Display Predefined Plots

This option makes use of The Unscrambler's many predefined result plots. After each analysis you can choose to see an overview plot of the most important results by pressing View. The **Plot** menu then consists of the appropriate result plots for the type of analysis you have performed. You can also access the results plots from **File - Open** at any time.

Plot Information

The Unscrambler gives a lot of information about the data in the current plot. If the **Plot ID** is turned on, a line at the bottom of the plot displays basic information. Toggle the Plot ID on and off using **View - Plot ID**. The table below shows some typical ways of identifying plots

Plot ID syntax

Plot type	Typical ID line	Explanation
Score plot, 2D Scatter	Alcohol, X-expl: 70%, 14% Y-expl: 29%, 28%	The results file is Alcohol. The explained X-variance is 70% for PC 1 and 14% for PC 2. The explained Y-variance is 29% for PC 1 and 28% for PC 2.
Loading plot, line	Octane, PC(X-expl, Y-expl): 1(70%,29%)	The results file is Octane. The explained X-variance is 70% and the explained Y-variance is 29% for PC 1.
Predicted vs. Measured	Alcohol, (Y-var, PC): (Methanol,3) (Methanol,3)	The results file is Alcohol. The predicted vs. measured results for the Y-variable Methanol is plotted using 3 PCs.

Other information about the plotted data such as data source, explanation of colors and symbols, etc., may also be shown in a separate window using **Window - Identification**. These windows are dockable views.

Use **View - Plot Statistics** to display the most relevant statistical measures.

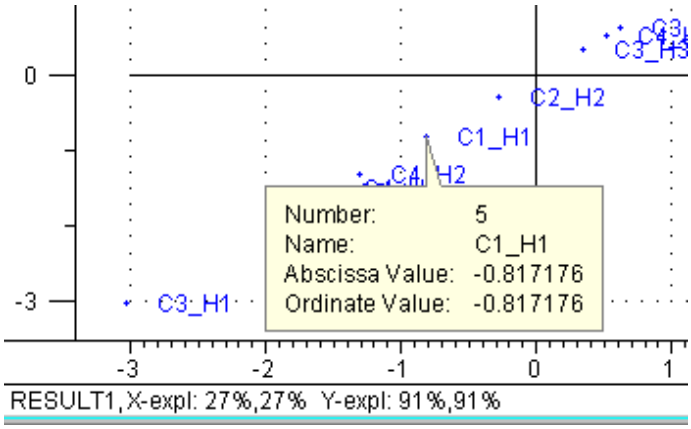
Information on each object in the plot can be displayed simply by letting the mouse cursor rest on the object in the plot. A brief explanation of the data point then appears. Click with the left mouse button to display more detailed information about the data object.

Point Details

In addition to the general information available about the whole plot, you may also display specific details regarding one particular point. This is done as follows:

- ***Rest the cursor*** close to a data point – the **point number** is displayed.
- ***Click on the point*** – a small **box** containing point number, point name and point coordinates is displayed as shown in the figure below.

Point Details are displayed by clicking on a data point



Use of Colors

There are three pre-set color schemes in The Unscrambler; Black background, White background and Greytones. You can change the color on any of the items of the Viewer. This is done through **File - System Setup - Viewer - Define colors…**. It is possible to use different color schemes for the screen and the printer.

For the printer, scheme Greytones is recommended if you have a black and white printer. You may modify the color scheme and choose your own grey levels.

Note that also other items than the background and the axis (foreground) differ in the preset color schemes; see below for details:

The Unscrambler color schemes

Item	Black background	White background
Foreground	White	Black
Curve 1	Cyan	Blue
Curve 2	Magenta	Red
Curve 3	Yellow	Green
Curve 4	Light blue	Light blue
Curve 5	Bright green	Brown
etc…		

It is also possible to set the color for a specific item. The changes will be shown on the preview screen.

Dockable Views

The Unscrambler shows different kinds of information in dockable views. A dockable view is a window that "floats" on the desktop and which can be "glued" to the edges of the Unscrambler workspace at wish, hence the term "dockable".

Dockable views are toggled on and off in the **Window** or **View** menu. Dockable Views in the **Window** menu are **Identification** and **Warning List**, in the **View** menu **Outlier List**.

Click the title bar of the dockable view to drag it around the screen. The shape of the view changes when you get close to the edge of the Unscrambler workplace. When you release the mouse button, the view is glued to the edge. To move it again, click inside the docked view and drag it away. When you get outside or well inside the edges of the Unscrambler workspace, the shape changes again and it has become a floating window.

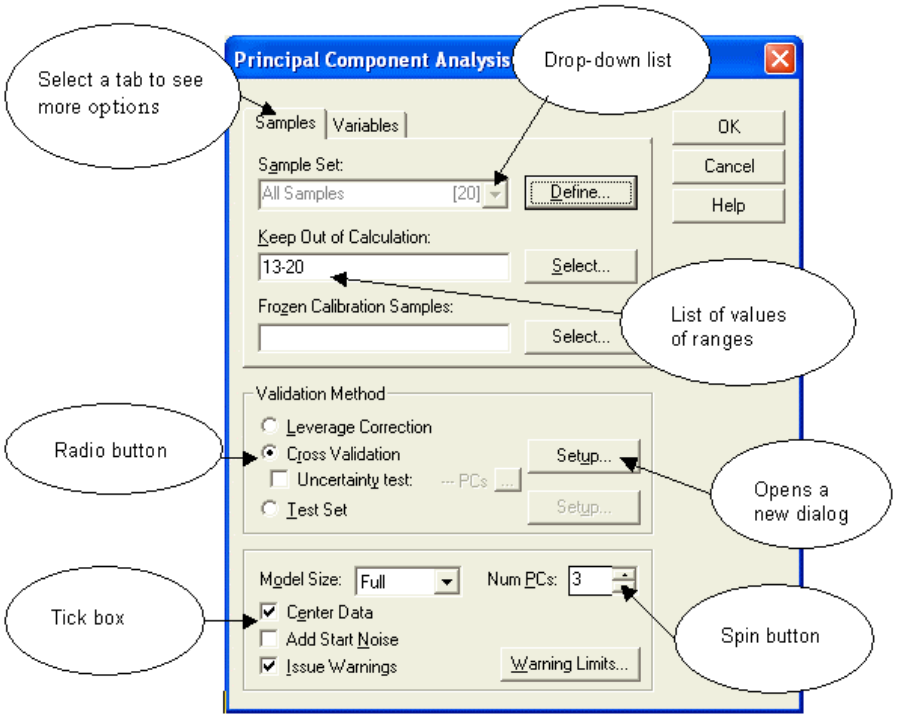
Dialogs and Wizards

Dialogs and wizards are the elements of the Unscrambler user interface that allow you to give detailed instructions to the program. A ***dialog*** is a single box that may contain one or several sheets, where you choose some options and press OK when you are ready. A ***wizard*** is a series of dialogs organized in a sequence, that lets you proceed through the successive stages of a longer operation by means of Next and Back buttons.

Dialogs

When you are working in The Unscrambler, you will often have to enter information or make choices in order to be able to complete your project, such as specifying the names of files you want to work with or the sets which you want to analyze, or how many PCs you want to compute. This is done in dialogs, which will normally look something like the one pictured below:

Unscrambler dialog

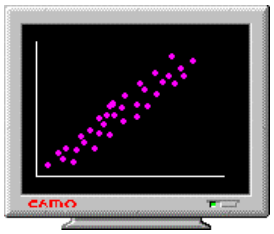


This particular dialog is the one you enter when you want to run a Principal Components Analysis on your data. Items that are predefined, such as sets, file filters, etc., are selected from a drop-down list. Ranges of samples or variables are entered as shown in the **Keep Out of Calculation** field in the figure. You can use a comma to separate two items in a field, and a hyphen to specify the whole range between two values.

Options which are mutually exclusive are selected via radio buttons. Tick boxes are used to select multiple options. For example, you may center data and issue warnings at the same time.

Plot Preview in Plot Dialogs

Plot Preview



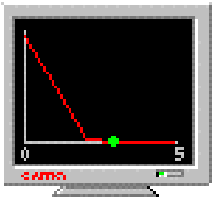
Plot dialogs show you a preview of any plot type you are about to make (like in the figure above), enabling you to check that your choice of plot was correct. You do however have to keep in mind that this is not a preview of your own data, it just shows the general shape of the plot and indicates in which sub-view the plot will be displayed. Double-clicking on the preview screen allows you to change the size of the plot window in the Viewer.

Extracted File Information

Dialogs involving management of files on disk have an information field at the bottom. The Unscrambler searches the files for information that tells you more about the contents of the file. This information typically includes:

Type of file	
File name	Size of the matrices
Directory name	Set information
Creator	Weighting information
Date of creation	Calibration method
Software version	Validation method

Preview screen for true residual variance curve



A preview screen (see figure above) in the information area of the file dialogs shows the true residual variance curve for the currently selected model whenever you select a result file that has the residual variance saved. The dot shows the optimal number of components suggested by The Unscrambler.

You also have access to the variance as a numerical table, and the warnings from the information field of the dialogs.

Wizards

A wizard is a set of dialogs which are predefined by The Unscrambler as belonging together, i.e., the choices made in one dialog naturally lead you to the next. Dialogs in a wizard are connected with Next and Back buttons, which allow you to switch back and forth between dialogs within the wizard. The Next button in a specific dialog will only be enabled when you have filled in all necessary information; with the help of the Back button, you can however go back and change this information at a later stage. In the last dialog of the wizard, the Next button is substituted with the button Finish.

Getting Help in The Unscrambler

When working in The Unscrambler, you may get help on any feature by accessing the Help system or by using tooltips for toolbar buttons.

The Help System

The Help system has been implemented to give you the help and advice you need when you are working with The Unscrambler. Help is available on the following topics:

- Use of the dialogs
- Use of the methods
- Interpretation of plots

Access the Help system at any time by pressing the <F1> button or clicking on the Help button in the dialogs. The Help file is automatically opened at the appropriate topic.

Get Help on a specific menu option or button on the toolbar by activating the **Help button** and clicking on the feature you wish to read about.

You may also open the help system by selecting **Help - The Unscrambler Help Topics** or clicking on ; this displays all the contents of the Help file. From there you can click your way to the items you are interested in, just as you would open a book. Use the Index tab to search for keywords.

Several levels of help are available. Click on underlined words to follow built-in links to related help topics.

Read more about The Unscrambler Help System and its menu options in chapter p. 297.

Tooltips

Whenever you let the cursor rest on one of The Unscrambler's buttons or icons, a small yellow label pops up to tell you its function. This is the quickest way to learn the functions of toolbar buttons.

Communication with Other Software and Instruments

Like most Unscrambler users, you are probably already using many different programs in your daily work. You might collect data using computers linked to your instruments or via data acquisition packages, write your reports using word processors, or use presentation programs to prepare lectures. The Unscrambler can interact with these and many other applications in many ways.

The first chapter hereafter gives you an overview of the systems The Unscrambler is compatible with.

The next chapter contains a list of useful tips, while the last one lists all menu options that allow you to transfer data or models between The Unscrambler and other applications.

Compatibility

Overview of the systems The Unscrambler is compatible with.

Windows® Compatibility

The Unscrambler runs under Windows 95, Windows 98, Windows NT (3.51 or later), Windows 2000 and Windows XP.

Data may be copied from The Unscrambler to other Windows-based applications (or the other way round) by means of Copy / Paste or drag'n drop (see section Useful Tips for Import / Export for more details).

You may also copy graphs from The Unscrambler to other Windows-based applications, either directly, or by saving a plot as bitmap which can then be opened in another application.

Overview of Compatible Formats

The external file formats compatible for import and export to / from The Unscrambler are listed in the table below.

Formats compatible for Import / Export

File Format	Import	Import 3-D	Export
ASCII	Yes	Yes	Data
ASCII-MOD	-	-	Model
LOTUS	Yes	-	-
EXCEL	Yes	Yes	-
JCAMP-DX	Yes	Yes	Data
Vision	-	-	Model
Tracker	Yes	-	Model
NSAS	Yes	-	Model
APC	Yes	-	-

GRAMS	Yes	-	-
Matlab	Yes	Yes	Data
Guided Wave	Yes	-	-
Indico	Yes	-	-
Hitachi F3D	-	Yes	-
MVACDF	Yes	-	Data

More details about Instrument compatibility are given in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

Useful Tips for Import / Export

The easiest way to share information between applications is to **copy** data tables and plots to the clipboard and **paste** them from the clipboard into other applications.

Other ways to do it are:

- **Export** data, models or result matrices;
- **Import** data;
- Transfer data from **spreadsheets**;
- Transfer **plots.**

Exporting Data from The Unscrambler to Other Programs

Sometimes, you want to use data tables from The Unscrambler in your reports. The contents of the data table may be raw data or model results (e.g. regression coefficients).

The procedures for exporting to a word processor and a spreadsheet are different.

Transferring Your Data to a Word Processor

Mark the data you want to transfer and select **Edit - Copy**. Go to the word processor and select **Edit - Paste**. The data is now transferred with sample and variable names. Select the data and convert them to a table (e.g. **Table - Convert text to table** in Word), and format this table as you wish to make it look nice.

Transferring Your Data to a Spreadsheet

Export the data to an ASCII file (select **File - Export** and set the file type to ASCII. The ASCII file should be exported as a block file with no name qualifiers).

Go to your spreadsheet and open the ASCII file. In Excel, a wizard will guide you through the process. In step 2 you should change the delimiter to the one you chose in the **Export** dialog, which is a comma by default.

You can also use the clipboard (copy and paste) to transfer data to a spreadsheet, but this will only transfer the data, not the names.

Exporting a Model in ASCII-MOD Format

All results necessary to define a model can be written in the ASCII-MOD format, allowing another program to read in everything necessary to reproduce the model you have made in The Unscrambler. You can also export the model to NSAS or Vision format, etc. This option allows you to export an Unscrambler model to another program, using the ASCII-MOD file format.

Go to **File - Export Model** and select the kind of result file you want to export. Type in the name of the file you want to export in the **Export…** dialog, or click the Browse button to get a list of all available models.

The ASCII-MOD file structure is described in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

Exporting a Result Matrix

You can also export any result matrix to another file format, e.g. as an ASCII file.

A data table can be written from an Editor to disk in different file formats, e.g. JCAMP-DX (a file format used by many spectroscopic software programs). Plain ASCII file format is the most commonly used, as it is easily read by most other programs.

You must import result matrices into an Editor using **File - Import - Unscrambler Results** before you can write them to disk in another file format.

Importing Data into The Unscrambler Using Drag'n Drop

The Drag'n drop feature is a very fast way to transfer data between Windows applications. You can use Drag'n drop to import data into The Unscrambler from applications such as Microsoft Excel.

Note: Data tables can only be transferred as "text", i.e. it is not possible to link or embed them in other applications (i.e. you cannot use OLE or DDE to transfer them).

Transferring Data from Spreadsheets into The Unscrambler

The easiest way to transfer data from Excel and Lotus spreadsheets is to have both programs open at the same time and use Drag'n drop (see section Importing Data into The Unscrambler Using Drag'n Drop).

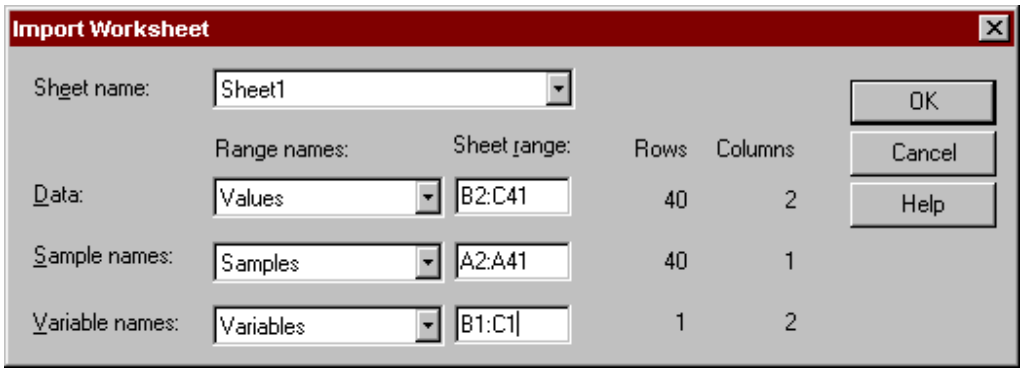
However, there are times when you do not want to open an extra program and still want to import the spreadsheet file directly from disk.

For instance, you may not have Excel on your PC, but you would still like to import data from an Excel file that you got from a colleague into The Unscrambler.

In those cases, it is smart to have used the Names function of the spreadsheet program and given the different matrices a name. You should also do this for sample and variable names.

If The Unscrambler detects that you have named some areas of the spreadsheet, you can quickly select the name from the range list instead of typing the cell area. Do this from the **Import from Worksheet** dialog which pops up after choosing **File - Import - Excel** (or Lotus).

The Import from Worksheet dialog with range names



Note: The source file containing the spreadsheet from which you want to import should not be opened by another application (e.g. Excel) while you are performing the import.

Transferring Unscrambler plots to Another Application

You can use copy and paste to transfer a plot from The Unscrambler Viewer to another program. Click on the plot you want to transfer and select **Edit - Copy**, or select **Edit - Copy All** if you want to copy all plots together. Then go to the other application and select **Edit - Paste**.

The plot can be transferred either as a bitmap or as a meta-file (picture). The latter option gives the best quality, but may result in very large files in Word, especially if the plot has many objects (many samples and/or variables, using symbols layout, etc.). You select the appropriate option in the **Viewer** sheet of the **File - System Setup** dialog.

Another possibility is to save the plot using **File - Save Plot** (or right-click on the plot and select **Save Plot**). This allows you to choose among a few different file formats, which later on can be opened in the application of your choice.

A Special Case: Transferring Table Plots

Table plots (e.g. ANOVA table) are nothing but characters and numbers displayed in a graphical interface. Thus, if you copy a table plot and paste it into another application, you will get the following results:

- In a spreadsheet, e.g. Excel: A table, with row and column names;
- In a word processor, e.g. Word: A tabulated series of words and values, which can easily be converted into a table (see section Transferring Your Data to a Word Processor).

Import / Export in Practice

Menu options for import and export with various formats.

How To Import Results or Data (2-D)

With the **File - Import** options, you can import a data table from another program, as well as results from an Unscrambler model. Once you have made all the necessary specifications in the **Import** and **Import from Data Set** dialogs, a new Editor, which contains the imported data, will be created in The Unscrambler.

Read more about the **File - Import** menu options in chapter File - Import p. 50.

How To Import Results or Data (3-D)

With the **File - Import 3-D** options, you can import a three-way data table from another program, as well as three-way result arrays from an Unscrambler model. Once you have made all the necessary specifications in the dialogs, a new Editor, which contains the imported three-way data, will be created in The Unscrambler.

Read more about the **File - Import 3-D** menu options in chapter File - Import 3-D p. 66.

How To Export Data

With the **File - Export** option, you can export data from an Unscrambler data table to an external program. In the **Export** dialog, you will have to select the required export format, and you will then access a new dialog where you may specify the parameters of the export.

Read more about the **File - Export** menu options in chapter File - Export p. 71.

How To Export Models

With the **File - Export Model** options, you can export an Unscrambler model to an external format so that the model can be used by an instrument or another software for prediction or classification. An export dialog allows you to specify the details of what to export, depending on the export format.

Read more about the **File - Export Model** menu options in File - Export Model p. 74.

The Unscrambler Menu Options

The chapters that follow describe the detailed program operation with the help of the system of menu options available from the Unscrambler's Main window, Editor and Viewer.

These options are grouped into the following sub-menus:

The Unscrambler Menu System

Sub-menu	See description page…
The File Menu	45
The Edit Menu	119
The View Menu	151
The Plot Menu	175
The Modify Menu	217
The Task Menu	253
The Results Menu	289
The Window Menu	292
The Help Menu	297

In addition, the ***Design Wizard*** launched by File Menu options **File - New Design** and **File - Duplicate - As Modified Design**, is described in a chapter of its own starting p. 97.

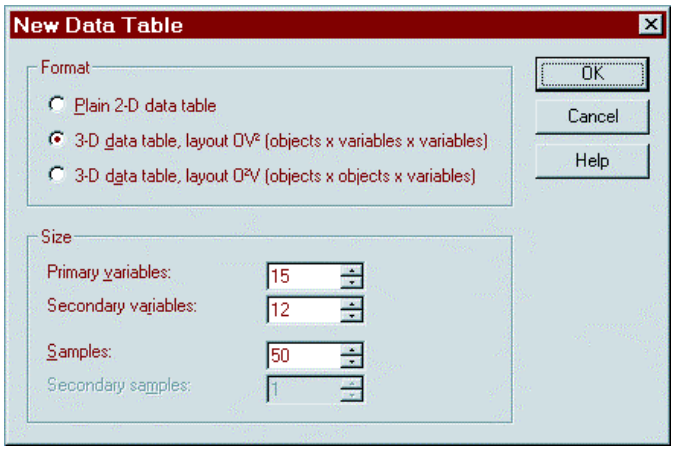
The File Menu

File - New…

or **Ctrl+N**

You use this option if you want to create a new data table by typing the data directly into the Editor or by importing foreign files. You enter a dialog called **New Data Table**, where you have a choice between three layouts for your data.

Dialog New Data Table, accessed from menu: File - New



Choose a layout (see below for more details) and fill in desired number of variables and samples.

Upon clicking **OK**, you enter an Editor window containing an empty data table with the specified size. Fill in the row names, column names and values for your data.

Plain 2-D data table

Specify the size of the table by filling in the fields Variables and Samples. Type in the desired number, or use the spin button to tune the value up and down.

File - New: 3-D data table, layout OV²

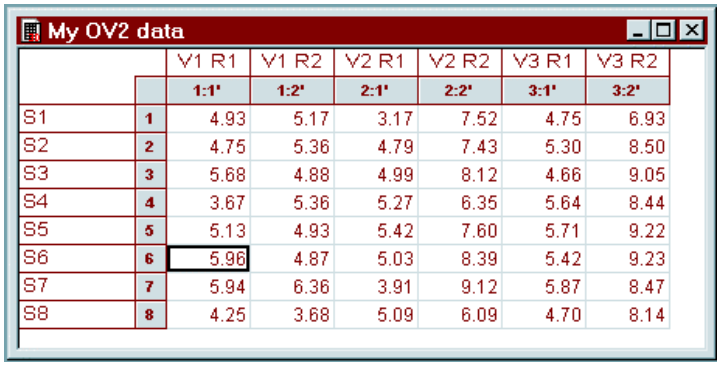
Specify the size of the table by filling in the fields Primary variables, Secondary variables and Samples. Type in the desired number, or use the spin button to tune the value up and down.

Fill in the names of your samples by double-clicking on the left margin, where sample names are displayed.

Fill in the names of your variables by double-clicking on the upper margin, where variable names are displayed. Variable names consist of two parts: Primary Var Name, Secondary Var name. The two parts are separated by a hyphen ("-"). If you try to enter something else in the Variable Name field, an error message will be displayed, prompting you for a correct entry (see the **Invalid Format** dialog).

See the figure below for an example of the OV^2 layout.

OV2 data table in the Editor



		V1 R1	V1 R2	V2 R1	V2 R2	V3 R1	V3 R2
		1:1'	1:2'	2:1'	2:2'	3:1'	3:2'
S1	1	4.93	5.17	3.17	7.52	4.75	6.93
S2	2	4.75	5.36	4.79	7.43	5.30	8.50
S3	3	5.68	4.88	4.99	8.12	4.66	9.05
S4	4	3.67	5.36	5.27	6.35	5.64	8.44
S5	5	5.13	4.93	5.42	7.60	5.71	9.22
S6	6	5.96	4.87	5.03	8.39	5.42	9.23
S7	7	5.94	6.36	3.91	9.12	5.87	8.47
S8	8	4.25	3.68	5.09	6.09	4.70	8.14

File - New: 3-D data table, layout O^2V

Specify the size of the table by filling in the fields Variables, Primary samples and Secondary samples. Type in the desired number, or use the spin button to tune the value up and down.

Fill in the names of your samples by double-clicking on the left margin, where sample names are displayed. Sample names consist of two parts: Primary Sam Name, Secondary Sam name. The two parts are separated by a hyphen ("-"). If you try to enter something else in the Sample Name field, an error message will be displayed, prompting you for a correct entry (see the **Invalid Format** dialog).

Fill in the names of your variables by double-clicking on the upper margin, where variable names are displayed.

See the figure below for an example of the O^2V layout.

O2V data table in the Editor

My O2V data

		V1	V2	V3	V4	V5	V6
		1'	2'	3'	4'	5'	6'
S1 R1	1:1	5.62	0.00	9.10	4.49	3.91	6.44
S1 R2	1:2	5.96	9.60	5.95	2.68	5.43	1.67
S2 R1	2:1	6.28	3.62	3.78	2.89	10.00	7.94
S2 R2	2:2	4.26	4.62	1.86	5.90	3.87	9.18
S3 R1	3:1	3.29	2.04	7.12	3.55	6.90	4.99
S3 R2	3:2	5.74	5.15	5.83	2.14	2.47	4.59
S4 R1	4:1	2.60	8.48	8.79	4.39	1.83	4.28
S4 R2	4:2	4.67	4.77	3.02	2.88	6.33	6.37

File - New: 3-D data table, variable and sample names

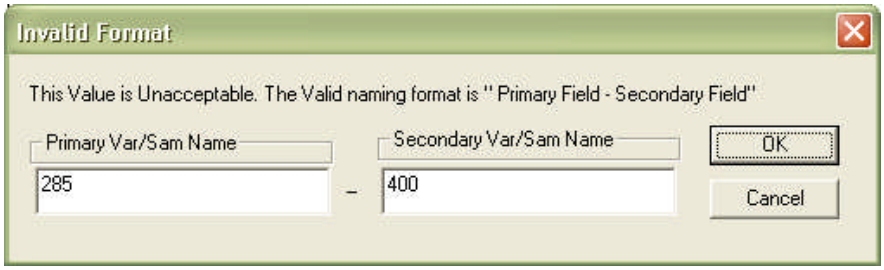
The columns of a 3-D data table with layout OV^2 are combinations of Primary and Secondary variables. Thus Variable names consist of two parts, referring resp. to Primary Var and Secondary Var Name.

Similarly, the rows of a 3-D data table with layout O^2V are combinations of Primary and Secondary samples. Thus Sample names consist of two parts, referring resp. to Primary Sam and Secondary Sam Name.

The two parts of the name are separated by a hyphen ("-").

Upon invalid entry in one of the two-part name fields, the **Invalid Format** dialog prompts you for a correctly built name, as shown below.

The Invalid Format dialog

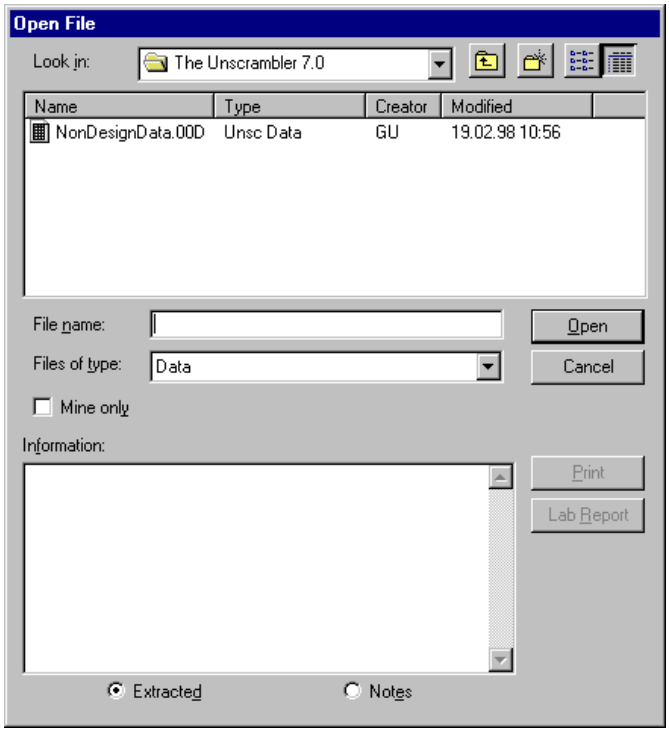


File - Open…

or **Ctrl+O**

This option opens an existing file in a new window. If it is a data table, an Editor document appears; if it is a result file, a predefined Viewer appears. You enter the dialog **Open File**, as shown below.

Dialog: Open File



From the drop-down list in the field Look in, select the folder which contains the file you wish to open. The field below will be updated to display all files in the folder of the type specified in the field Files of type. You can change the type of file with the drop-down list in this field.

If you know the name of the file you want to open, you can type it directly into the field File name, otherwise select the appropriate file from the displayed list. Press Open.

At the bottom of the dialog, an information field displays information about the selected file. You can switch between extracted information, i.e. a brief summary of the file, or the notes for the file, using the radio buttons below the field.

If you want a print-out of the information, press the Print button to the right of the field. The Lab Report button directly below it lets you print the lab report for the file.

File - Close…

This option closes the current data table or result file. If you have not previously saved changes to the document, The Unscrambler asks if you want to save the document before you close it.

Note: If you close a window without saving, you will lose all changes you did not save previously. This includes “invisible” changes in the file log which are made automatically every time you run an analysis.

File - Save

or **Ctrl+S**

Saves the active file, displayed in an Editor or a Viewer, with the name, location, and file format you previously set in the **Save As** dialog. When you save a document for the first time, The Unscrambler displays the **Save As** dialog.

If you want to change the name, location, or file format of an existing document, you must choose the **File - Save As** command.

File - Save As…

Lets you save the contents of the current window as a new file without destroying the original file. Specify the new location, name, and type of file.

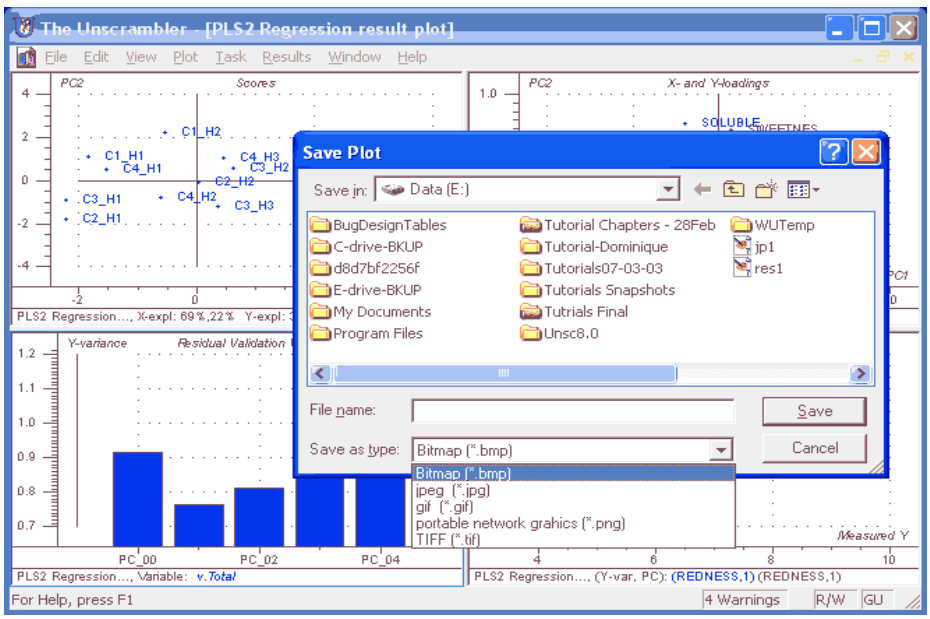
File - Save Plot

Access this option from the context-sensitive menu (right mouse-click) **Save Plot…** or from **File - Save Plot…** when a plot is displayed in the Viewer. This option leads you to the **Save Plot** dialog where you can save a plot as an image file in five different formats: *.bmp, *.jpg, *.gif, *.png and *.tif.

Example:

The X-and Y-loadings plot of a PLS regression analysis can be saved by right-clicking on the plot and choosing the desired file format in the **Save Plot** dialog.

Dialog: Save Plot, in use on a PLS regression result plot



File - Import

This option lets you import data from an external data file. This may be a file from an earlier version of The Unscrambler or one with a different format, e.g. Excel or ASCII.

Note: The Unscrambler looks for files with the expected extension only. You have to rename the file extension if the file you want to import has another.

How to Import Data

When you have chosen which kind of file you want to import from the **Import** sub-menu, you enter the first dialog: **Import Target**. Once you have selected your import target and clicked OK you enter the **Import** dialog.

Import Target

This dialog appears only if the currently active document is a non-designed data table. It gives you 3 choices regarding your import target:

- New data table
- Current data table (from cursor position)
- Current data table (from origo)

Make your choice and click OK.

The imported data is inserted as the leftmost variables or the upper samples when you choose to insert them from origo.

Note: Importing data into the current Editor will overwrite any cells that are covered by the imported data area. If you do not want to overwrite these cells, use the Insert or Append commands to insert new samples/variables before you begin importing data.

Import Dialog

Once you have selected your import target and clicked OK you enter the **Import** dialog, which is identical to the **Open File** dialog, except that the buttons Print and Lab Report are not available. Select the file which contains the data that you want to import and press Import. Dialogs, differing according to the type of file, allow you to select which matrices to import and give any other information The Unscrambler needs to import the data.

Import With Drag'n Drop

Instead of going via the **File-Import** menu, you can import data by using Drag'n drop. You simply mark data in another Windows program and drag it into The Unscrambler's Workspace or into an existing Editor document. If you drop the data table onto the Workspace, an Editor will be opened automatically.

You select whether you want to insert the data as columns or rows. The columns or rows are appended at the end of the existing data table.

You may also overwrite the existing data in the Editor. The area that is going to be overwritten is marked by a frame.

Supported Formats for Import

The Unscrambler lets you import data from the following formats:

- Unscrambler Results (see File - Import - Unscrambler Results … p.51);
- Unscrambler Data (see File - Import - Unscrambler Data … p.52);
- Unscrambler5 Results (see File - Import - U5 Results … p.53);
- Unscrambler5 Data (see File - Import - U5 Data … p.53);
- Unscrambler ASCII files (see File - Import - Unscrambler ASCII … p.53);
- Flat / Flat wide ASCII files (see File - Import - ASCII … p.53);
- Lotus files (see File - Import - Lotus … p.55);
- Excel files (see File - Import - Excel … p.55);
- Database (see File - Import - Database … p.56);
- JCAMP-DX files (see File - Import - JCAMP-DX p.59);
- Tracker files (see File - Import - Tracker … p.61);
- NSAS files (see File - Import - NSAS … p.61);
- APC files (see File - Import - APC … p.61);
- GRAMS files (see File - Import - GRAMS … p.61);
- Matlab files (see File - Import - Matlab … p.61);
- MVACDF (see File - Import - MVACDF … p.62);
- Guided Wave files (see File - Import - CLASS-PA & SpectrOn … p.63);
- Indico files (see File - Import - Indico … p.64);
- Files from Brimrose instruments (see File - Import - BFF3 … p.64);
- User Defined Import (UDI) (see File - Import - User Defined Import (UDI) … p.65).

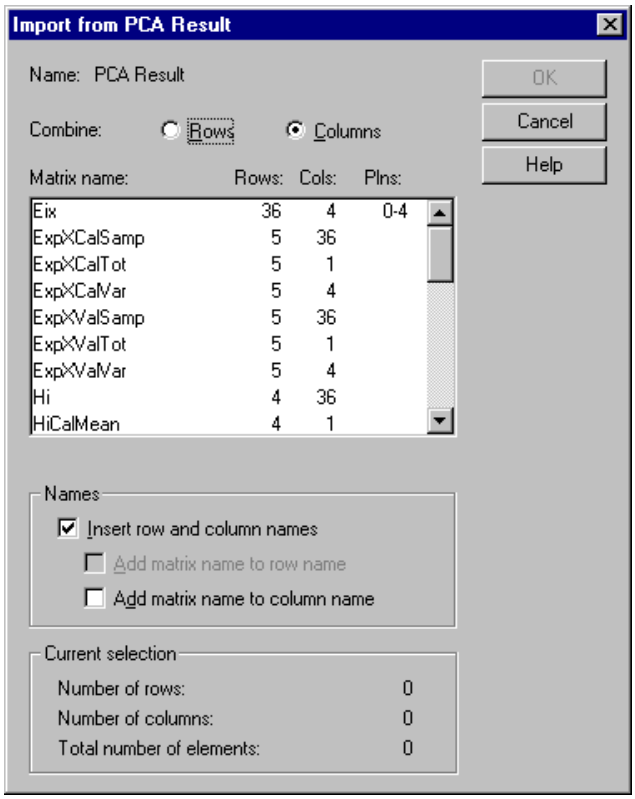
File - Import - Unscrambler Results …

Ctrl + U

You can read result files made by earlier versions of The Unscrambler into the Editor to study their numerical values by selecting the file-type and file you want to import in the **Import** dialog.

You then enter the **Import from (X)** dialog (where (X) represents the result file type), see the figure below for an example. You select the matrices you want to import from the matrix list. See the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices, for a list of all matrices used in The Unscrambler.

Dialog: Import from PCA Result



First, you choose whether you want to import rows or columns by clicking the appropriate radio button. Then, select the matrices you want to import from the file. Several matrices can be imported together, by combining either rows or columns. Matrices that will not match the ones already chosen will be grayed out.

You can import several matrices either by rows or columns, depending on whether your matrices contain the same number of variables (row-wise import) or samples (column-wise import).

If the matrices contain sample and/or variable names, you can import them as well by selecting the appropriate option box.

Note: Some matrices have more planes, one for each PC calculated. Normally, you should choose the same plane for all.

The planes may be PCs, groups, etc., according to which matrix you want to import. Several planes can be imported at once by entering a range, e.g. '3-6'.

If you import several matrices and want to import another plane than the first, you specify the correct plane number after you have marked the first matrix.

File - Import - Unscrambler Data …

You can read data files made by earlier versions of The Unscrambler into the Editor to study their numerical values by selecting the file-type and file you want to import in the **Import** dialog.

You then enter the **Import from (X)** dialog (where (X) represents the data file type). You select the matrices you want to import from the matrix list. See the Technical References chapter, which is available as a .PDF file

from CAMO's web site www.camo.com/TheUnscrambler/Appendices, for a list of all matrices used in The Unscrambler.

First, you choose whether you want to import rows or columns by clicking the appropriate radio button. Then, select the matrices you want to import from the file. Several matrices can be imported together, by combining either rows or columns. Matrices that will not match the ones already chosen will be grayed out.

You can import several matrices either by rows or columns, depending on whether your matrices contain the same number of variables (row-wise import) or samples (column-wise import).

If the matrices contain sample and/or variable names, you can import them as well by selecting the appropriate option box.

File - Import - U5 Results …

Imports results files from earlier versions of The Unscrambler (versions 3.0 - 5.5). If the file you want to import contains several matrices, a dialog pops up to let you specify which matrices you want to import.

Note: The Unscrambler recognizes the extensions: .UNM, .UNP, and .CLA. Rename your files if they have other extensions.

File - Import - U5 Data …

Imports data files from earlier versions of The Unscrambler (versions 3.0 - 5.5). If the file you want to import contains several matrices, a dialog pops up to let you specify which matrices you want to import.

Note: The Unscrambler recognizes the extensions: .UNS, .UNM, .UNP, and .CLA. Rename your files if they have other extensions.

File - Import - Unscrambler ASCII …

Imports files from The Unscrambler version 1.0 - 2.3e. The file format is described in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices.

Use Flat/Flat Wide ASCII import if you have ASCII files you want to import from other programs.

File - Import - ASCII …

You may import data from ASCII files with different formats, provided that you specify as much as you know about the nature of the ASCII file you want to import. This is done in the field File format in the dialog **Import ASCII**, see the figure below, which you enter when you click Import in the **Import** dialog. An ASCII file can be ***flat*** or ***flat wide***.

Note: Files with extension .csv can now be imported using **File - Import - ASCII**.

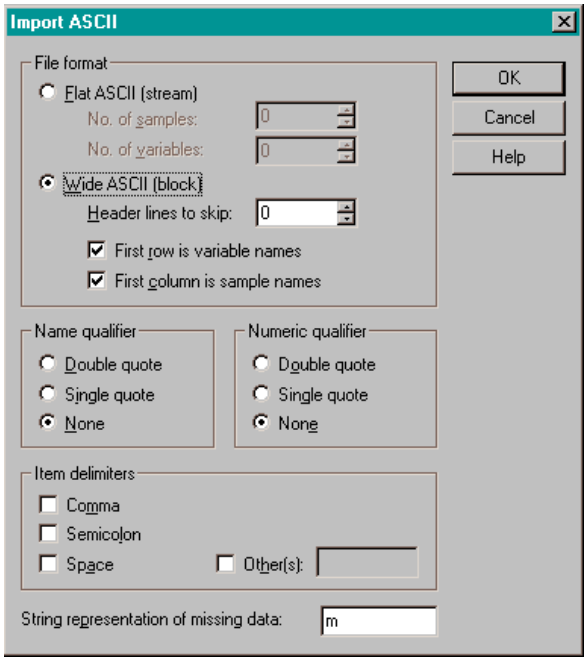
Flat ASCII (Stream) files

are simply strings of numbers with no delimiters. It is therefore vital that you know the exact size of the matrix. The Unscrambler reads the first sample with as many numbers (i.e. variables) as you have specified in the variables field, then proceeds to the next sample. These files cannot contain names, only numbers.

Flat Wide ASCII (Block) files

use a paragraph character to denote the end of each sample. The file may also have header lines giving information about its contents. You must enter the number of header lines, or they may be imported into the matrix as “data”.

Dialog: Import ASCII



If sample and/or variable names occur in the first column or the first row, you can also import those by selecting the box in the File format section.

Text or numbers may occur within single or double quotes in the file you import from. In the fields Name qualifier and Numeric qualifier respectively you should specify the quotes that are used, to make the import more secure. However, it is now also possible to import names without any quotes, even if those names may contain some spaces. This applies both to sample / variable names and category variable levels.

Note: If names are not enclosed in quotes in your ASCII file, they should not contain any spaces if you select “space” as item delimiter (see Item delimiters below).

Numbers may be delimited by different characters in different ASCII files. Specify which delimiter is used in the file you want to import, using the field Item delimiters. You may choose “Comma”, “Semicolon”, “Space” or specify another delimiter, e.g. “\”.

Note: Carriage Return, Line Feed and Tabulation are not among the available delimiters in the dialog. They are default item delimiters, and will automatically be recognized as such. Do not specify them in the “Other(s)” field!

You must also enter the character string used to represent missing data in the ASCII file you want to import in the box String representation of missing data. They will be replaced and displayed as “m” in the Editor.

File - Import - Lotus …

You can import data from Lotus 1-2-3 files of .WK3 and .WK4 type.

Remember to close the file in Lotus before trying to import it.

You can enter the range to import manually, specifying the upper left cell and the lower right cell, eg. B2:H34. All cells lying within this rectangle are then imported.

Do this for the data range, and also for the sample and variable names, if they exist in the Lotus file.

Note: You must clear the sample and variable names fields if you do not want to import such names.

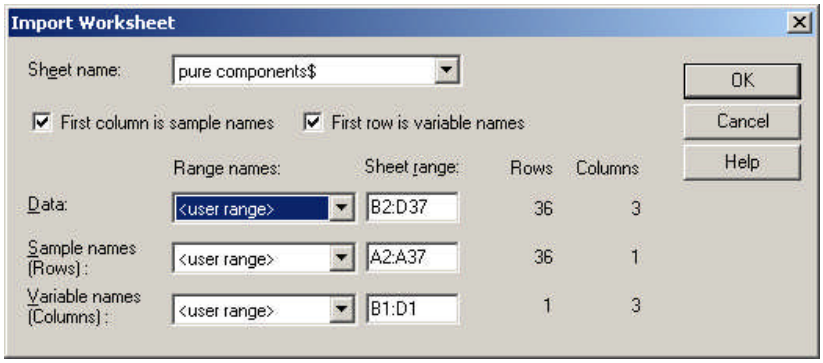
File - Import - Excel …

You can import data from Microsoft Excel versions 5, 7 and 8 (Excel 97) workbooks and version 4.0 worksheets. The Excel files must have the extension .XLS.

Remember to close the file in Excel before trying to import it.

When you select to import data from an Excel file in the **Import** dialog, you enter a new dialog, **Import Worksheet** shown below. An Excel workbook may contain several worksheets. Select the worksheet that contains the matrix you want to import from the drop-down menu Sheet name.

Dialog: Import Worksheet



The check-boxes right under Sheet name take care of the most common cases where First column contains all sample names or First row contains all variable names. Un-tick them if not relevant.

The rest of the dialog box lets you specify where to find the data to be imported. It takes advantage of the "Name" function in Excel, which lets you allocate a name to a certain area, or group of cells (in Excel, use **Insert - Name - Define** to define a range and give it a name).

All ranges that have been defined with names in the selected Excel sheet are listed under Range names. The sheet range is updated automatically if you select a range name. You can also enter the range manually, specifying the upper left cell and the lower right cell, eg. B2:H34. All cells lying within this rectangle are then imported.

Select the appropriate ranges as described above for the data values, as well as for the sample and variable names, if relevant.

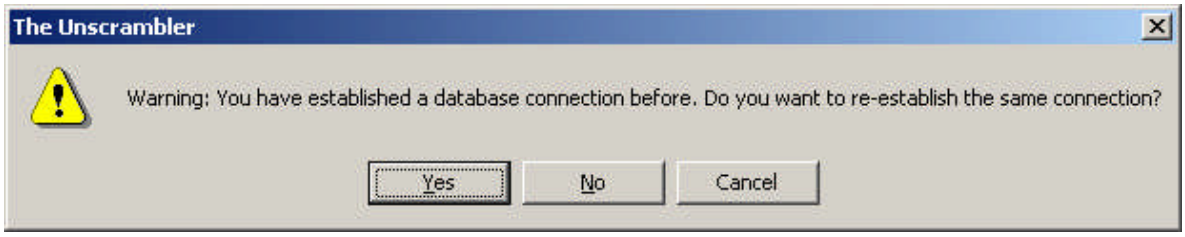
Note: You must clear the sample and variable names fields if you do not want to import such names.

File - Import - Database …

You may import data from a database into The Unscrambler's Editor. Since there are many possible database platforms and the data structure may be complex, you need to go through several dialogs in order to specify the import:

1. Data Link Properties dialog;
2. SQL Query dialog.

If you use **File - Import - Database …** several times without logging off from The Unscrambler, the following message box will appear:


The Unscrambler
Warning: You have established a database connection before. Do you want to re-establish the same connection?
Yes
No
Cancel

If you click Cancel, the **Data Link Properties** dialog is bypassed, keeping the same connection details as previously, and you access the directly.

Click No in order to access the **Data Link Properties** dialog and specify new connection details.

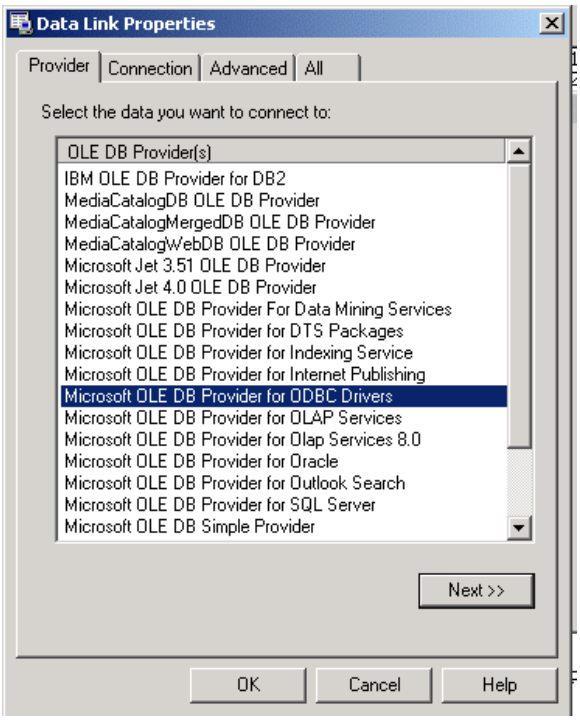
The Cancel button cancels the **File - Import - Database …** command.

Note: The **Data Link Properties** dialog is a standard Windows dialog. Depending on your local language setup, this dialog may be displayed in another language than English. The name of the dialog will be different, the fields will have a different text, but the layout and meaning of all fields will be the same as described hereafter.
The next two sections describe the standard stages you need to go through in order to establish a connection from The Unscrambler to a database. For addidional information, click Help; this will start the Microsoft help system related to the current sheet in the **Data Link Properties** dialog.

Data Link Properties Dialog: Provider Sheet

In the Provider sheet of the **Data Link Properties** dialog, select the database provider you want to import from.

Dialog: Data Link Properties, Provider sheet

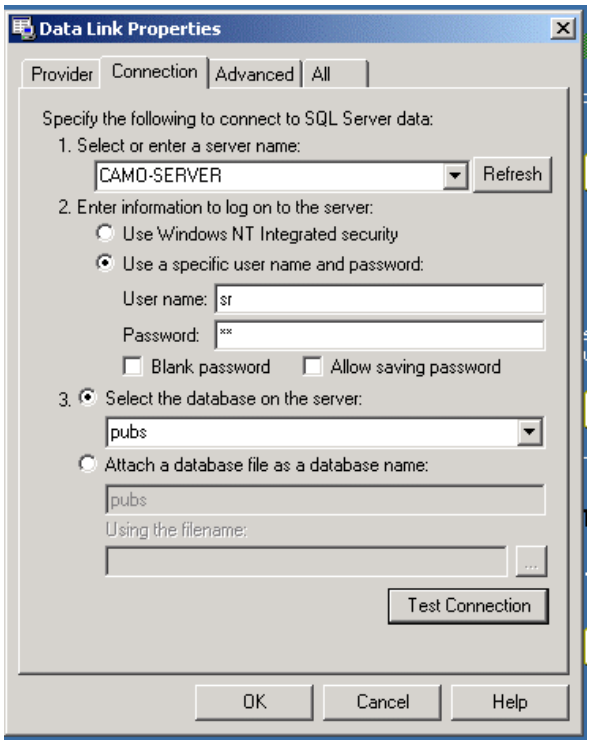

Data Link Properties
Provider
Connection
Advanced
All
Select the data you want to connect to:
OLE DB Provider(s)
IBM OLE DB Provider for DB2
MediaCatalogDB OLE DB Provider
MediaCatalogMergedDB OLE DB Provider
MediaCatalogWebDB OLE DB Provider
Microsoft Jet 3.51 OLE DB Provider
Microsoft Jet 4.0 OLE DB Provider
Microsoft OLE DB Provider For Data Mining Services
Microsoft OLE DB Provider for DTS Packages
Microsoft OLE DB Provider for Indexing Service
Microsoft OLE DB Provider for Internet Publishing
Microsoft OLE DB Provider for ODBC Drivers
Microsoft OLE DB Provider for OLAP Services
Microsoft OLE DB Provider for Olap Services 8.0
Microsoft OLE DB Provider for Oracle
Microsoft OLE DB Provider for Outlook Search
Microsoft OLE DB Provider for SQL Server
Microsoft OLE DB Simple Provider
Next >>
OK
Cancel
Help

Hit Next to shift to the next dialog sheet, “Connection”.

Data Link Properties Dialog: Connection Sheet

In the Connection sheet of the **Data Link Properties** dialog, you locate the desired database from the proper server and specify the security settings for logging on to the database.

Dialog: Data Link Properties, Connection sheet



Specify the three fields:

1. Select or enter a server name: this combo box lists all servers available on your network.

2. Enter information to log on to the server: specify the access mode, either through Windows NT authentication or with a user name and password. Tick off "Allow saving password" if you wish to save the connection details.

3. Select the database on the server: this combo box lists all databases available on the selected server. Choose the database from which you want to import.

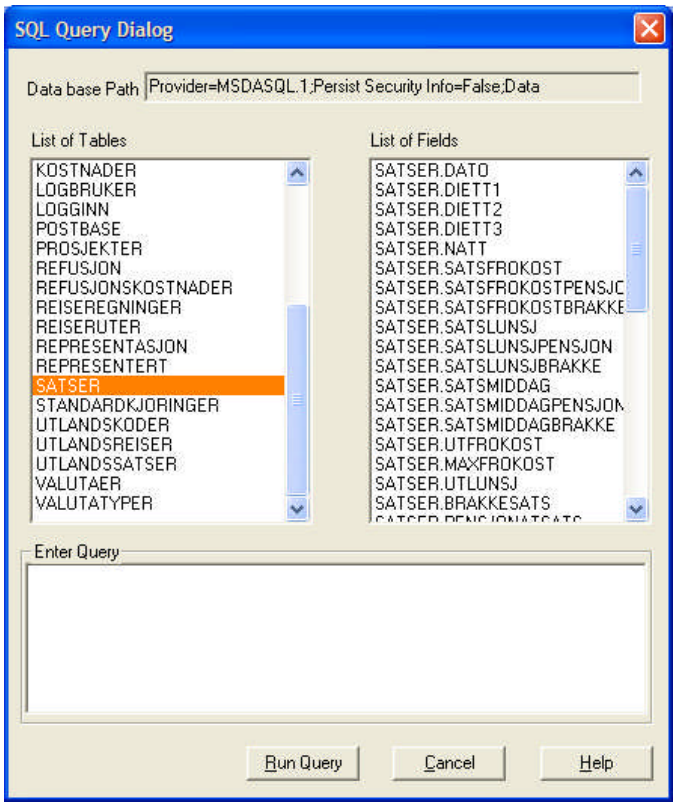
Once everything is specified, hit Test Connection to check whether you have successfully established contact with the desired database.

Click OK to access the next dialog, **SQL Query Dialog**.

SQL Query Dialog

The **SQL Query Dialog** allows you to enter an SQL query manually.

SQL Query Dialog



From the List of tables, select the data table you want to access. The List of fields to the right is then updated accordingly. If you double click on the table name, it will be displayed in the Enter Query area below.

Type in your query (involving available fields) in the Enter Query edit box.

Click the Run Query button to import the data into The Unscrambler.

To abort the import, click Cancel.

Note:

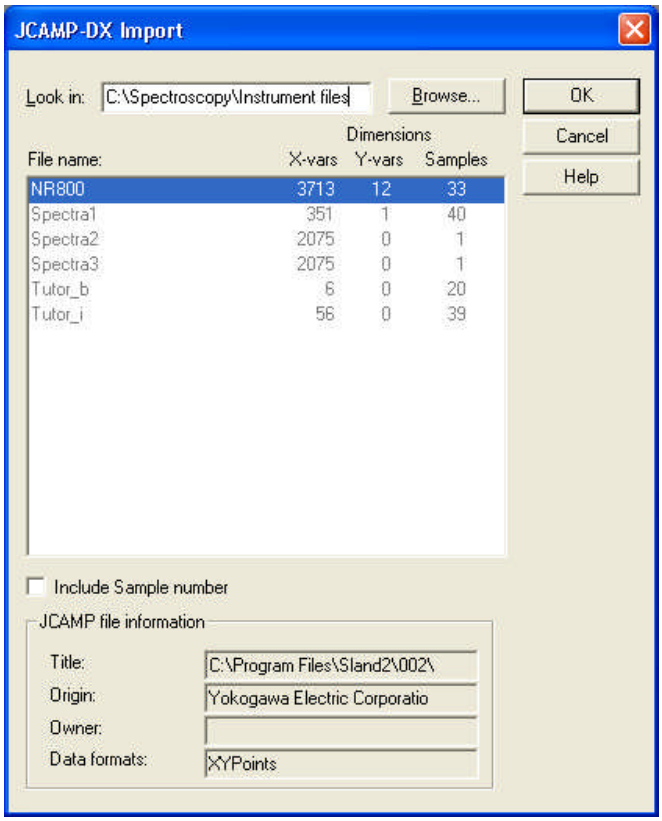
If you are not familiar with the Standard Query Language (SQL) widely used for extracting data from a database, you should contact your database administrator for help regarding how to formulate your query.

File - Import - JCAMP-DX …

You may import one or several JCAMP-DX files into The Unscrambler's Editor. More details regarding JCAMP files are given in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices.

Select the files you want to import from the file list in the dialog **JCAMP-DX Import** or use the Browse button to get a list of available files. The different files must have the same number of X-variables and the same contents in the Y-matrix to allow simultaneous import. All files that do not conform to the contents of the first selected file are grayed out.

Dialog: JCAMP-DX Import



You can select a group of files by pressing the <Shift> key while you click on the files you want to import.

Option Include Sample number will import the sample number together with the sample name. The sample number is specified in field “Sample description” of the JCAMP file:

##SAMPLE DESCRIPTION= [name] $$ [number]

By default, this option is not active: only the sample names are imported.

Sample names after import - with / without sample number

Sample number	Original sample name	Sample name with “Include Sample number”	Sample name without
…	…	…	…
23	BWX98	BWX98 23	BWX98
24	BWX98	BWX98 24	BWX98
25	BWY01	BWY01 25	BWY01
26	BWY01	BWY01 26	BWY01
27	BWY02	BWY02 27	BWY02
28	BWY02	BWY02 28	BWY02
…	…	…	…

Note: Sample names will only be imported if they are present in the source JCAMP-DX file.

The field JCAMP File Information at the bottom displays summary information about the last file selected in the file list.

File - Import - Tracker …

Through this option you can import Tracker files which are written by Multispec instruments from Foss Electric.

Several predefined Sets, e.g. Sets for calibration samples, are created automatically during import of the file.

File - Import - NSAS …

You enter the **Import** dialog, where you select the NSAS file you want to import from the list of files in the folder.

NSAS Data Import will read information in the NSAS data file which has no natural place in The Unscrambler's file format into the Instrument Info block (**File - Properties**) under specific keywords. Similarly, NSAS/Vision Model Export will look for a relevant subset of these keywords and, if found, it will place the values in the corresponding places in the NSAS/Vision Model file.

File - Import - APC …

This option is used to import files generated by APC, a package used with some Infralyzer instruments. The data are stored in an observation file (*.OBS) and additional header information is stored in a header file (*.HDR). Both files must be present.

The variables Sets Filters and Constituents are defined. Product Name and File Description is saved as instrument parameters in **File - Properties**.

File - Import - GRAMS …

Here, you may import files generated by GRAMS, a software package used with some Galactic instruments. You choose the appropriate file in the dialog **GRAMS32 Import**.

The Variable Sets Filters and Constituents are defined. Product Name and File Description is saved as instrument parameters in **File - Properties**.

File - Import - Matlab …

This option lets you import data from Matlab formatted files created in Matlab versions 5.x to 7.0.

To Save Data for Importing

Use the **save** command in Matlab:

- either "**save** destinationfilename var1 var2 …",
- or "save destinationfilename" to save all variables in the workspace.

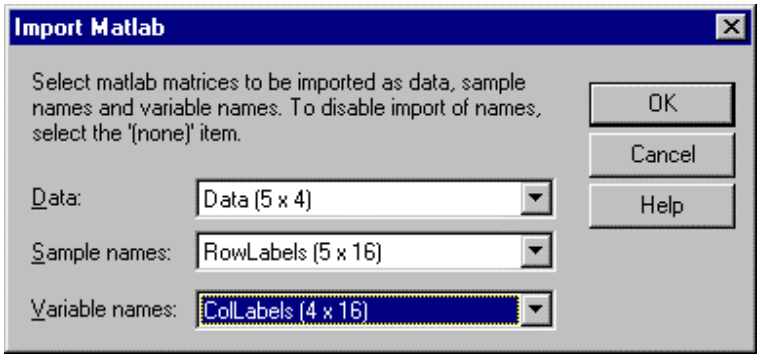
This will create a Matlab formatted .mat file. For more help on using the save command, type **help save** in Matlab.

To Import into The Unscrambler

To import the file in The Unscrambler, select **File - Import - Matlab**. Select the destination filename in The Unscrambler to get the **Import Matlab** dialog box.

Select which selections represent the Data, Sample names and Variable names. The sample name and variable name variables must match the corresponding dimension of the data variable (for example, 5 rows and 4 columns in the figure below) or they will not be displayed in the pull-down choice menus for sample and variable names.

Import Matlab dialog


Import Matlab
Select matlab matrices to be imported as data, sample names and variable names. To disable import of names, select the '(none)' item.
OK
Cancel
Help
Data:
Data (5 x 4)
Sample names:
RowLabels (5 x 16)
Variable names:
ColLabels (4 x 16)

Matlab variables representing sample and variable names must be character arrays.

What Cannot be Converted

The following cannot be imported from Matlab to The Unscrambler:

1. Matrices containing imaginary numbers,
2. Cells arrays,
3. Structures,
4. Sparse matrices.

File - Import - MVACDF …

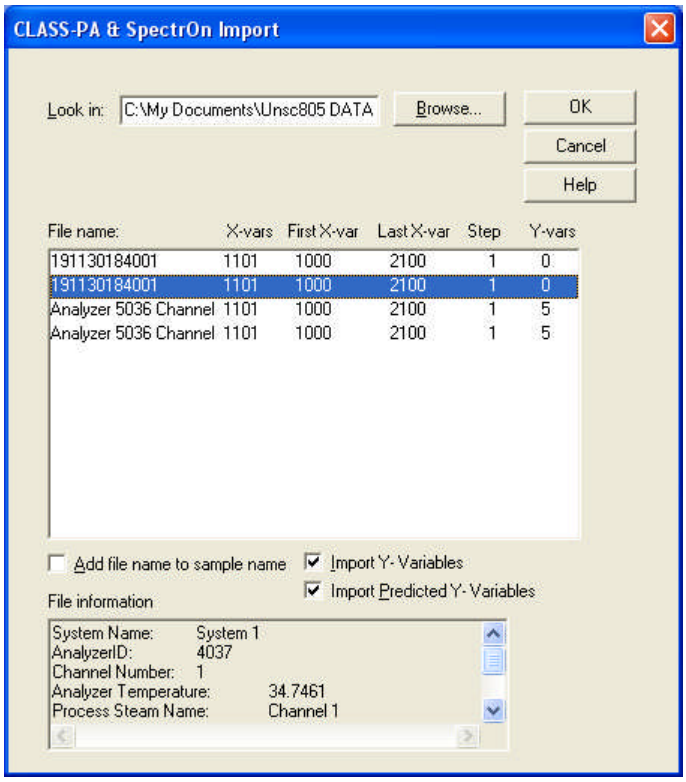
In The Unscrambler 7.6 a new import format was implemented to answer the specific needs of one of our major Unscrambler users. This format is called MVACDF and is accessible from the menu **File - Import - MVACDF.**

Note: If you also collect your data in a particular format and would like The Unscrambler to be compatible to this format, please take contact with us.

File - Import - CLASS-PA & SpectrOn …

This option lets you import data from Guided Wave files with the following formats: *.asc, *.scn and *.autoscan.

Dialog: CLASS-PA & SpectrOn Import



The **CLASS-PA & SpectrOn Import** dialog box displays a list of files from which you may import Guided Wave data. File name, number of X-variables, names of the First and Last X-variables, Step and number of Y-variables are displayed for each file.

If necessary, click the Browse button close to the Look in: field in order to access files from a different folder.

Once you have selected a file from the list, information about the file contents is displayed in the File information field at the bottom, helping you check that you have chosen the correct file.

Multiple selections are possible, using Shift + Click or Ctrl + Click.

You may select 3 additional options:

- Add file name to sample name
- Import Y-Variables
- Import Predicted Y-Variables

Click OK to validate your choices and perform the import.

File - Import - Indico …

This option lets you import data from files created with the Analytical Spectral Device software Indico. Source files with the following formats are supported: *.asd, .001, .002, .3456 etc (any number).

The **Indico Import** dialog box displays a list of files from which you may import Indico data. File name, number of X-variables, names of the First and Last X-variables and Step are displayed for each file.

If necessary, click the Browse button close to the Look in: field in order to access files from a different folder.

Once you have selected a file from the list, information about the file contents is displayed in the File information field at the bottom, helping you check that you have chosen the correct file.

Multiple selections are possible, using Shift + Click or Ctrl + Click.

You may select one additional option:

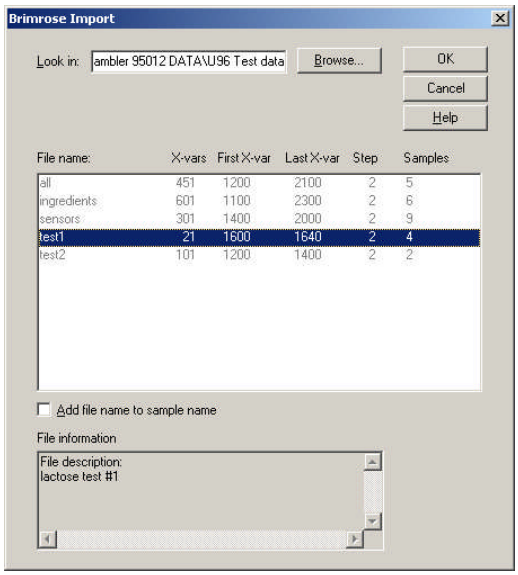
- Add file name to sample name

Click OK to validate your choices and perform the import.

File - Import - BFF3 …

This option lets you import data from Brimrose instrument files. Brimrose source files with the *.dat format are supported.

Dialog: Brimrose Import



The **Brimrose Import** dialog box displays a list of files from which you may import Brimrose data. If necessary, click the Browse button close to the Look in: field in order to access files from a different folder.

File name, number of X-variables, wavelengths for the First and Last X-variables, Step and number of Samples are displayed for each file.

NB- "Step" is the increment in wavelength (or wave number) between two successive variables. The following relationship should be true:

First X-var + Step*Xvars = Last X-var

Example:

Look up file “test1” in the dialog snapshot above. It has 21 X-variables, starting at 1600 and ending at 1640, with a step of 2, verifying the relationship

1600 + 2*21 = 1640

Once you have selected a file from the list, information about the file contents is displayed in the File information field at the bottom, helping you check that you have chosen the correct file.

Multiple selections are NOT possible.

You may select the additional option at the bottom:

- Add file name to sample name

Click OK to validate your choices and perform the import.

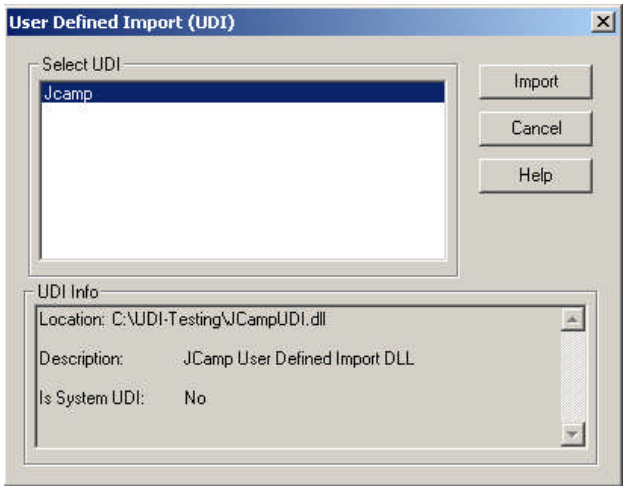
File - Import - User Defined Import (UDI) …

This option lets you import data from external formats which are not directly supported by The Unscrambler, using a DLL Plug-in approach.

This works in a similar way to User-defined transformations and analyses (see User-defined Transformation), and requires the desired import format to have been registered in The Unscrambler by your system administrator (see Related Topics below).

The command launches the **User Defined Import (UDI)** dialog which lets you choose the desired UDI from a list, then access the Import dialog.

Dialog: User Defined Import (UDI)



Select the required UDI from the list, then look up the UDI Info field to check whether this UDI indeed refers to the Import format you are looking for.

If OK, click Import to access the Import dialog.

If the UDI you are looking for does not appear on the list, check with your system administrator whether it has been registered in The Unscrambler (see Related Topics below).

Note:

Clicking Import starts the User Defined Import procedure. For obvious reasons, The Unscrambler Help system does not cover that stage of the import. Should you encounter any trouble while defining or performing the import, contact your system administrator or the person responsible for that particular UDI.

Related Topics

Register a new UDI: File - UDI - Register New UDI

Un-register an existing UDI: File - UDI - Unregister UDI

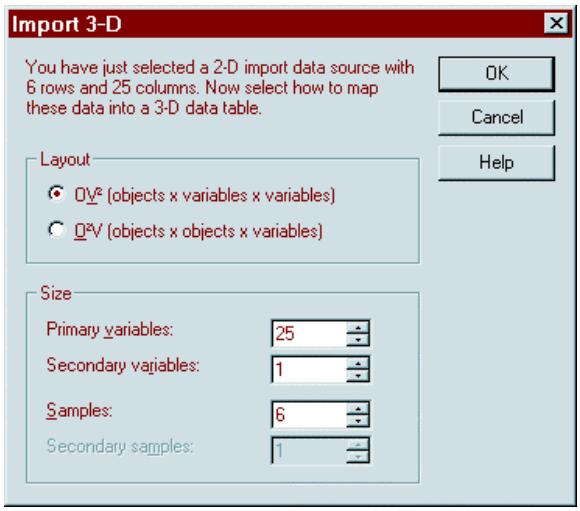
File - Import 3-D

The menu option **File - Import 3-D** allows you to import 3-D data from various sources.

Choose the relevant type of file; you enter the Import browser where you can search for and select the desired source file (only files of relevant type appear in the list). Select file and click Import.

The Import 3-D Dialog

Dialog: Import 3-D



In the **Import 3-D** dialog, no matter which source you imported from, you can specify the 3-D layout of your choice. Choose between layouts OV^2 and O^2V, then select the relevant numbers of samples and variables of each type (Primary - Secondary).

Supported Formats for Import 3-D

The Unscrambler lets you import data from the following formats:

- Unscrambler Results (see File - Import 3-D - Unscrambler Results …);
- Flat / Flat wide ASCII files (see File - Import 3-D - ASCII …);
- Excel files (see File - Import 3-D - Excel …);
- JCAMP-DX files (see File - Import 3-D - JCAMP-DX …);
- Matlab files (see File - Import 3-D - Matlab …);
- F3D files (see File - Import 3-D - F3D …).

Drag'n Drop 3-D

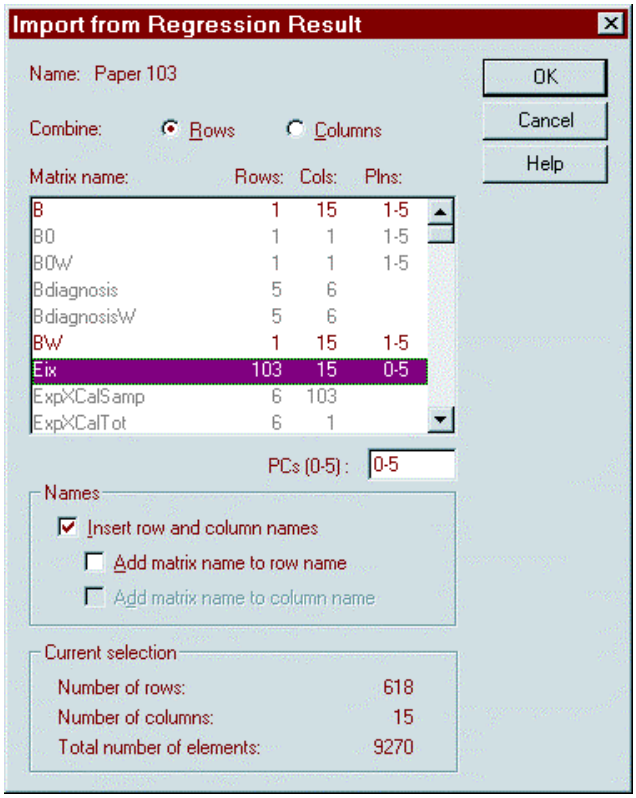
A selection from a 3-D data table can be dragged in the usual way. If you choose to drop it into an empty spot of the workspace, this will create a new table of type 2-D data.

Otherwise, you may drag and drop selections between 2-D and 3-D tables, provided that the dimensions are consistent. For instance, dragging and dropping rows into an OV^2 table is OK, but dropping columns into an OV^2 table is not allowed because they would not fit into the Primary / Secondary variable structure.

File - Import 3-D - Unscrambler Results …

The **Import from … Result** dialog allows you to choose one or several result matrices to be stored as three-way data. The figure below shows an example where the Eix (X-residuals) matrix has been selected from a Regression model, with 103 samples (“Rows”), 15 variables (“Cols”) and 6 PCs (“Plns” standing for Planes).

Dialog: Import from ... Result



The text on top of the dialog box states the name of the Unscrambler result file you are importing from. On the figure above, the file name is “Paper 103”.

Below, choose whether to Combine Rows or Columns. This option plays a double role, as described in the “Details” sections hereafter.

Once you have chosen whether to combine Rows or Columns, select the matrix or matrices you want to import from the list displayed in the middle of the dialog box. If a selected matrix has several planes, remember to fill in the relevant PC number(s) in the PCs field (or the desired segments using the Segments field) below the list. You may enter either one value (e.g. “4”, meaning you want only PC4), several values separated by “,” (e.g. “0,4”, meaning you want PC0 and PC4), or a range (e.g. “1-4”, meaning you want PCs 1 to 4).

The last choice you have to make is Names. If you tick the box Insert row and column names, the names stored in the source matrix will be included in the new table. Tick the box Add matrix name to row name (when combining Rows) or Add matrix name to column name (when combining Columns) to get non-ambiguous names in the case of several source matrices.

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

Importing several matrices into the same data table

If you combine Rows, the first selected matrix determines the number of columns in the resulting table. All matrices with a different number of columns are grayed out; you may select additional matrices to be imported simultaneously among the remaining ones.

Likewise, if you combine Columns, the first selected matrix determines the number of rows in the resulting table, and only matrices with the same number of rows can be selected further.

Note: It is not recommended to import several planes from different matrices simultaneously, as this function has not been optimized to give a 3-way layout that makes sense.

Importing several planes from a matrix

Some result matrices (e.g. Eix in the figure previous page) consist of several rows, columns and planes. Usually the planes correspond to varying numbers of PCs in the model. For models where Martens' Uncertainty Test has been computed, some matrices have as many planes as cross-validation segments.

If you combine Rows, importing several planes from the same matrix will give you a 3-way data table with an O^2V layout. The original Columns of the matrix determine columns of the new table, while the original Rows determine Secondary samples and the Planes determine Primary samples.

If you combine Columns, importing several planes from the same matrix will give you a 3-way data table with an OV^2 layout. The original Rows of the matrix determine rows of the new table, while the original Columns determine Secondary variables and the Planes determine Primary variables.

File - Import 3-D - ASCII …

The **Import ASCII** dialog allows you to specify the parameters of the import from an ASCII source file. It is described in detail in The Unscrambler User Manual p. 208-209.

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

File - Import 3-D - Excel …

The **Import Worksheet** dialog allows you to specify the parameters of the import from an Excel source file. It is described in detail in The Unscrambler User Manual p. 210.

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

File - Import 3-D - JCAMP-DX …

For JCAMP-DX files, the standard file browser is replaced by the dialog **JCAMP-DX Import** where you may select one or several source files for the import. No additional parameters need to be specified since all relevant information is stored with the JCAMP-DX format. This dialog is described in detail in File - Import - JCAMP-DX.

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

File - Import 3-D - Matlab …

The **Import Matlab** dialog allows you to specify the parameters of the import from a Matlab source file (version 5.x up to 7.0). It is described in detail in File - Import - Matlab ….

Note: The Matlab import routine has been re-written completely to accommodate new features related to sample and variable names or 3-way data structure. As a consequence, source files in Matlab 4 or earlier format are no longer supported. If you are using an older version of Matlab, you may either upgrade to version 5.1 or use an ASCII format to exchange files with The Unscrambler.

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

File - Import 3-D - F3D …

Allows you to specify the parameters of the import from an F3D source file (Hitachi).

The **F3D Import** dialog box displays a list of files from which you may import spectral data. Each file is displayed with its File name and further characterized by the following parameters:

- Ex Start, Ex End, Ex Interval
- Em Start, Em End, Em Interval
- No Ex Var, No Em Var

If necessary, click the Browse button close to the Look in: field in order to access files from a different folder.

Once you have selected a file from the list, information about the file contents is displayed in the File information field at the bottom, helping you check that you have chosen the correct file.

Multiple selections are possible, using Shift + Click or Ctrl + Click.

You may select one additional option:

- Add file name to sample name

Click OK to access the next dialog **Import 3-D** where you will specify your 3-D table layout (see The Import 3-D Dialog for a detailed description).

File - UDI

This menu option is only available when logged on as Supervisor (see System Configuration in Practice for help on how to log on as Supervisor).

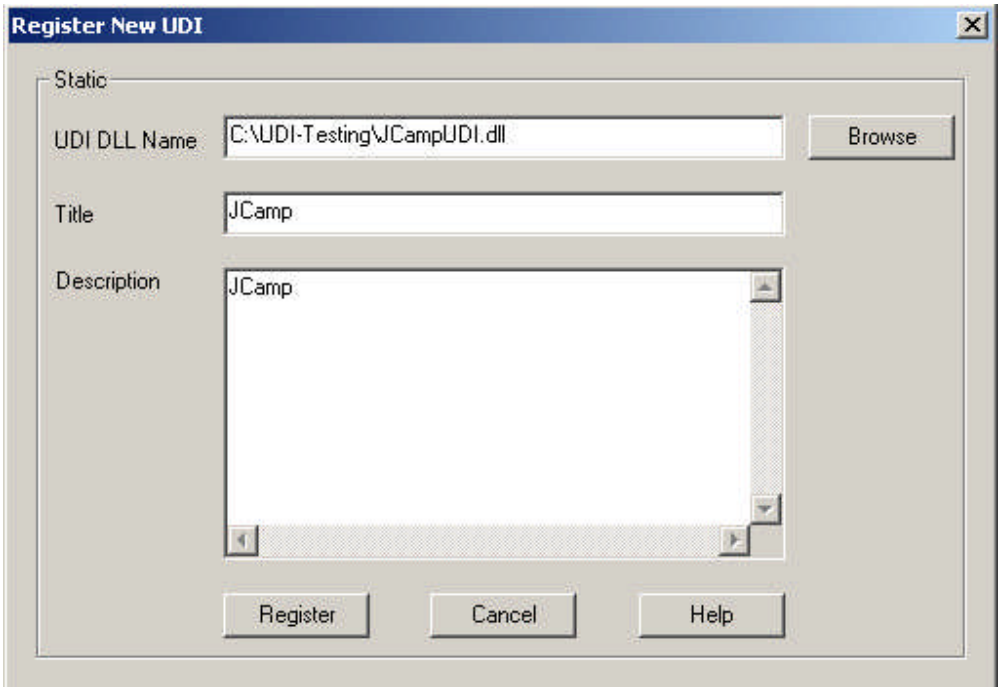
It allows you to register (i.e. “install”) a new UDI (User Defined Import format) or un-register a previously registered one, with the help of the following commands:

- File - UDI - Register New UDI;
- File - UDI - Unregister UDI.

File - UDI - Register New UDI

This command launches the **Register New UDI** plug-in dialog, where you can locate the relevant DLL and describe the new UDI for future use.

Register New UDI plug-in dialog



In the UDI DLL Name field, enter the full path and name of the .DLL file containing the UDI you wish to register. If necessary, click Browse to locate the file.

Type in a Title for the new UDI; this is the name that will identify the user-defined Import format for all Unscrambler users.

Type in a Description; make it detailed enough that other Unscrambler users reading this description will understand which Import format you are referring to.

When this is done, click Register; a new dialog box informs you that the new UDI has been successfully registered, then the **Register New UDI** dialog is activated again to allow you to register more UDIs.

When you have registered all your UDIs, click Cancel to exit.

Note:

Once a new UDI has been registered, it can be removed later on with the command **File - UDI - Unregister UDI** (Supervisor only).

File - UDI - Unregister UDI

This command launches the **UnRegister UDI** dialog, where you can remove a previously registered UDI.

File - Export…

This is a menu option which lets you export selected parts of a data matrix to an external file, in the format you define.

How to Export

When you select **File - Export**, you enter the **Export** dialog, which is similar to the **Open File** dialog (see File - Open…). Here, you must specify which file you want to export, and select the target format from the drop-down list Export as type. Then you press Export, upon which you will enter a dialog which will differ depending on what your chosen target format is.

Export 3-D

If you select a 3-D data table as source for an export, the result will have a 2-D matrix structure, even if the target for the export supports 3-way data.

Example: Upon exporting data from a 3-D data table to Matlab 5.1, you will get a two-dimensional array as a result.

More on How to Export

Chapter

File - Export Model gives further information about how models made with The Unscrambler can be exported.

The Unscrambler supports OLE Drag'n Drop, which may be a better way to export data to another Windows program. See chapter "Useful Tips for Import / Export" for more information.

Supported Formats for Export

The Unscrambler lets you export files as the following formats:

- Unscrambler ASCII;
- ASCII files;
- U5 data;
- JCAMP-DX files;
- Matlab files;
- MVACDF files.

Export: Unscrambler ASCII and U5 Data

The dialog **Export Unscrambler ASCII/Export Unscrambler 5** lets you define the sets you want to export.

Tick the box Export Y-Matrix if you want to include Y-variables in the file that you are exporting. Then, in the Sets field, define the appropriate Sample and X-Variable Sets. If you have chosen to export Y-matrix, you must also select a Y-Variable Set, otherwise, this option is not valid, i.e. grayed out. If you need to define new sets, click the appropriate Define button to enter the **Set Editor**, which allows you to define new sets or modify existing ones.

Export: ASCII Files

Many other programs can read ASCII files. This export option therefore is very useful if you want to work with the data table in another program.

You enter the **Export ASCII** dialog, where the Sets field lets you select the Sample and Variable Set you want to export. Click Define to define new sets in the **Set Editor**.

Then, specify whether to export as Flat or Flat Wide ASCII file in the File Format field. Flat ASCII files are a string of numbers with no delimiters. There are no characters to mark the different samples. The importing program has to know how many values to read before continuing to the next sample. Flat Wide ASCII files, on the other hand, have a paragraph character to denote the end of each sample.

Sample names and variable names can also be exported if you choose the format Flat Wide ASCII files. They will be placed in the first column and in the first row, respectively.

Decide whether text and numbers should occur within single or double quotes, or without quotes, in the fields Name Qualifier and Numeric Qualifier respectively. It is recommended to mark text with quotes and not mark numbers, because it makes it easier for importing programs to distinguish text and numbers.

Numbers may be delimited by different characters in different ASCII files. Specify which delimiter to use in the file you want to export in the Item Delimiters field.

Finally, specify how you want to represent missing data in the ASCII file you want to export in the field String Representation. The default option is ‘m’.

Export: JCAMP-DX Files

The JCAMP-DX format is read by many instrument softwares. This file format requires that the X-part of the data have numerical names, e.g. wavelengths.

Select the sets that make up the data matrix you want to write to the JCAMP-DX file in the Sets field. Define new sets in the **Set Editor** if the already existing sets do not contain the correct data.

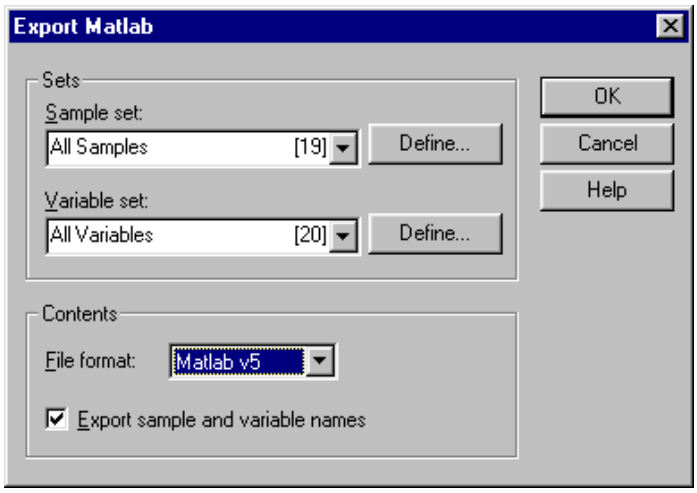
Then, in the field File Info, you enter information related to the JCAMP-DX file as a whole. You must choose between two JCAMP-DX formats: XYPoints and XYData. XYData requires that the distance between each variable's wavelength is the same throughout the whole X-Variable Set. XYData requires less hard disk space than XYPoints.

Enter information related to the samples in the Samples Info field. This information is saved with each sample.

Export: Matlab Files

The Unscrambler lets you export data tables to Matlab version 4 or version 5 formats including the sample names (row headings in The Unscrambler) and the variable names (column names in The Unscrambler).

Export Matlab dialog



The **Export Matlab** dialog box allows you to specify the data to be exported in terms of the Sample and Variables sets. All available sets are listed in the drop down boxes. If required new sets can be defined using the Define buttons.

In the Contents section, select the Matlab file version and optionally whether sample and variable names should be exported. If this option is selected then these names are stored in separate arrays within the export file as Matlab arrays do not support direct labeling.

The converted Unscrambler file is saved in a filename.mat file where filename represents what you have entered.

Reading the File in Matlab

To load the converted file, type "load *filename*" in the Matlab command window. If the data are exported without sample and variable names, the *filename.mat* file contains one variable called Matrix that contains the Unscrambler worksheet data. If the data are exported with sample and variable names, the *filename.mat* file contains 3 variables: Matrix, ObjLabels, and VarLabels where *ObjLabels* and *VarLabels* are character arrays that contain the row and column labels respectively.

Note: The variable names (**Matrix, VarLabels,** and **ObjLabels**) are the same in each exported Unscrambler file. Thus, if you want to load several converted Unscrambler files into Matlab, rename the variables in Matlab after each load command or they will be overwritten by subsequent import operations.

Missing Value Conversion

Missing values in an Unscrambler worksheet are converted to the number

-9.9730e+023.

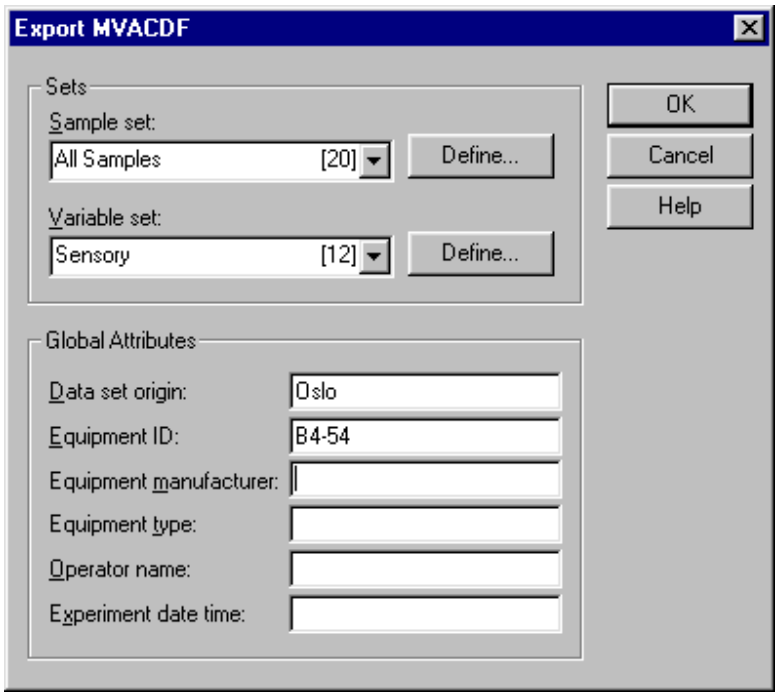
Category Variable Conversion

Category Variables are converted into integers.

Export: MVACDF Files

In The Unscrambler 7.6 a new export format was implemented to answer the specific needs of one of our major Unscrambler users. This format is called MVACDF. Upon choosing Type "MVACDF Files" in the **Export** dialog, you enter the **Export MVACDF** dialog shown below.

Export MVACDF dialog



Select the sets that make up the data matrix you want to write to the MVACDF file in the Sets field. Define new sets in the **Set Editor** if the already existing sets do not contain the correct data.

Then, in the field Global Attributes, you enter all other relevant details.

Note: If you also collect your data in a particular format and would like The Unscrambler to be compatible to this format, please take contact with us.

File - Export Model

The Unscrambler models can be exported to several formats.

See Chapter File - Export… for more information about how to export data.

How to Export Models

You need to specify the models which are to be exported, in the respective dialogs specific to each export format.

Supported Formats for Export Model

The Unscrambler lets you export files as the following formats:

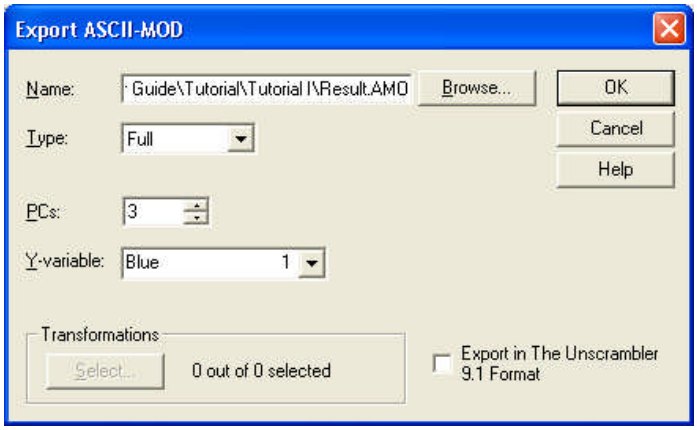
- ASCII-MOD (see File - Export Model - ASCII-MOD ...);
- U5 Model (see File - Export Model - U5 Model...);
- NSAS (see File - Export Model - NSAS ...);
- Vision (see File - Export Model - Vision ...);
- Tracker Model (see File - Export Model - Tracker ...).

File - Export Model - ASCII-MOD ...

A special ASCII file format has been developed to make it easier for you to convert Unscrambler results into other formats of your own choice. The file contains all necessary information for prediction and classification. See the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices, for a description of the ASCII-MOD file format.

When you choose to export this model, you enter the dialog **Export ASCII-MOD**. In the Name field, type the name of the file containing the ASCII-MOD data you want to export. If you do not remember the name, you can click the Browse button to get a list of all available models.

Dialog: Export ASCII-MOD (PLS1 model)



Choose between Full or Mini exports from the drop-down list in the Type field. Mini ASCII-MOD exports consist only of the B-coefficients from a regression model. Full ASCII-MOD means that all necessary model results are written to file.

Results up to and including the PC you specify in the PCs field are exported.

You can include a list of the transformations that have been performed on the data table from which the results originate. To do this, press Select in the Transformations field to enter the **Select Transformations** dialog, where you will find a list of all available transformations. Use the Select button to define which ones to include. You can also Select All or Select None.

For PLS1 models only, an extra option allows you to Export in The Unscrambler 9.1 Format. It has been introduced to ensure compatibility with some types of external instrument software and uses space delimitation instead of tabulations.

Note!

Use option "Export in The Unscrambler 9.1 format" if you intend to use the PLS1 model for prediction in instrument software from Yokogawa.

File - Export Model - U5 Model...

The Unscrambler saves the model in the old Unscrambler format used by the DOS versions. This way other software packages can still read the models you develop in The Unscrambler.

In the **Export U5 Model** dialog, specify the folder in which the U5 model should be stored in the Folder field. Use the Browse button if you do not remember the whole path and have to look at the tree structure.

In the field Model Name, you can enter five characters for the U5 model name. The three last letters are used by The Unscrambler to identify different U5 models.

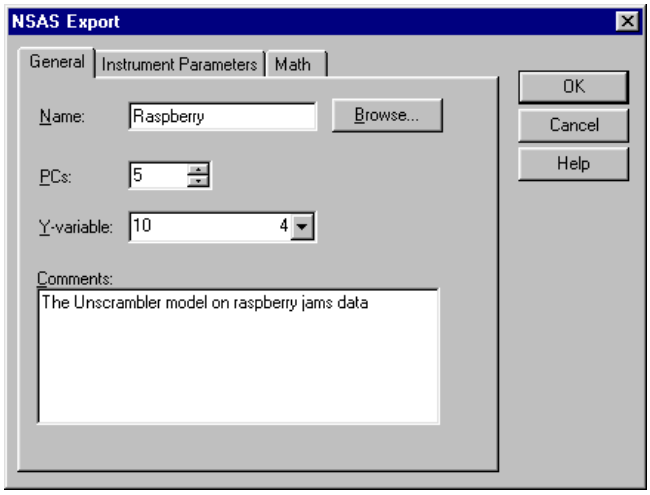
Check the box Include residuals to include the X-residuals (Eix) and Y-residuals (Fiy) in the exported model file.

File - Export Model - NSAS ...

This option exports the result file to NSAS format. The model can then be imported into the software package controlling your instrument. All necessary parameters for export to NSAS are not always found in the data and/or model files and must be entered by you.

The **NSAS Export** dialog contains three sheets; General, Instrument Parameters and Math.

NSAS Export dialog - General Sheet



NSAS Export Dialog: General Sheet

Specify the file name for the NSAS model file in the Name field. Use the Browse button if you want to change the folder in which the file should be stored. Then, select the number of PCs you want to use in the model in the PCs field. This is usually the optimal number of PCs.

In the Y-Variable field, select which Y-variable you want to export a model for. NSAS does only allow one Y-variable at a time. The number at the right end of the field shows which variable number it had in the Y-variable Set.

The Comments field allows you to write comments you want included in the model file.

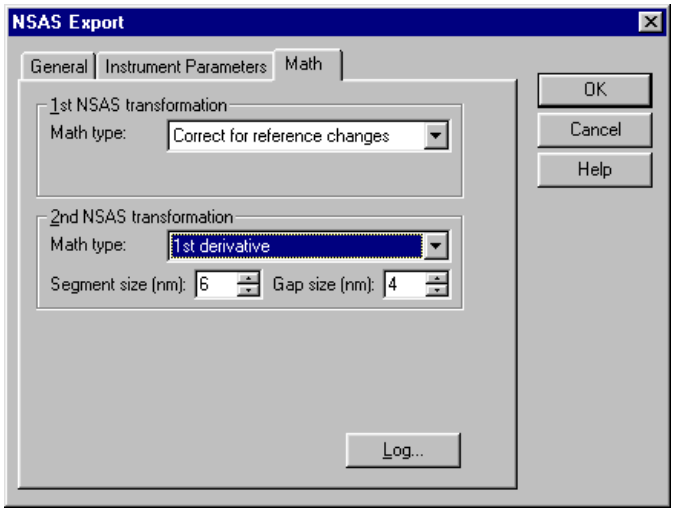
NSAS Export Dialog: Instrument Parameters Sheet

The instrument parameters which will be written to the NSAS file are displayed on this sheet. Most of the parameters are collected from the data and/or model file and cannot be changed.

NSAS Export Dialog: Math Sheet

This sheet is used to specify which transformations were applied to the data before calibration was performed. This is important if exported models are to be used for predictions, as spectra used as input to the prediction must undergo exactly the same transformations as the calibration spectra.

NSAS Export dialog - Math Sheet



NSAS allows for up to two transformations, specified in the fields 1st NSAS transformation and 2nd NSAS transformation respectively.

The first transformation is used for the sole purpose of indicating whether the spectra has been corrected for reference changes within the instrument or not. Choose Math type from the drop-down list.

The second transformation may be any NSAS math type, including None. Select from the drop-down list. For some of the math types, one or more of the parameters Segment size, Gap size, or Divisor point will be enabled. These will be written to the model file exactly as shown. Use the spin buttons to specify them.

Default values for the transformations are taken from the Instrument Information block in The Unscrambler's result file, which is again copied from The Unscrambler's data file. If the data file was originally imported from an NSAS data file, the Instrument Information block was created based on the information found in the NSAS data file, reflecting any transformations applied to the data before the NSAS data file was created. For this reason, you should not change any default values unless you are very confident in what you are doing.

Any transformation applied to the raw data using The Unscrambler must be manually specified. For more information about the correspondence between Unscrambler and NSAS transformations, see next chapter NSAS Transformations.

Press the Log button on this sheet to enter the Log where you can make notes about your export.

NSAS Transformations

When you have applied a transformation to your data using The Unscrambler prior to calibrating a model and exporting it to an NSAS/Vision model file, it is of vital importance that these transformations are flagged in the NSAS/Vision file to be able to perform correct predictions using the model. Unfortunately, there is not a simple one-to-one correspondence between the two programs, so some manual work is required by you.

Each NSAS/Vision transformation and the corresponding Unscrambler transformation is listed below. Note that a single NSAS/Vision transformation often corresponds to two Unscrambler transformations applied consecutively.

Important:

The Unscrambler always assumes parameters like segment sizes, gap sizes etc. to be expressed in number of data points (variables), whereas NSAS/Vision assumes these parameters to be expressed in wavelengths (nanometers). Therefore, you must multiply The Unscrambler's parameter with the difference in wavelength between two neighboring wavelengths in the original data table before you put it into the NSAS/Vision parameter field. An exception to this is NSAS/Vision Savitsky&Golay smoothing, which assumes number of data points as segment size, just like The Unscrambler. Vision Savitsky&Golay 1st and 2nd derivative assumes the segment size parameter to be expressed in number of data points for the smoothing part and in nanometers for the derivation part of the transformation.

NSAS/Vision transformations and corresponding Unscrambler transformations

NSAS Math Type	NSAS/Vision Math Type Name	Unscrambler Transform Name	Comments
1	N-point smooth	Smoothing, Moving Average	
2	Reflective energy	Spectroscopic, Absorbance to Reflectance + Compute: Multiply by 100.0	NSAS multiplies result by 100 to express it in %.
3	Kubelka-Munk	Smoothing, Moving average + Spectroscopic, Absorbance to Reflectance + Spectroscopic, Reflectance to Kubelka-Munk	
4	1st derivative	No equivalent (The Unscrambler's Norris Derivation gives similar results, but applies a slightly different smoothing, and scales (divides by number of points between segment centers).	NSAS/Vision derivation disregards distance between points or segment centers, ie. derivative results are "unscaled".
5	2nd derivative	No equivalent	As above
6	3rd derivative	No equivalent	As above
7	4th derivative	No equivalent	As above
8	Savitsky&Golay	Smoothing, Savitsky&Golay	2nd order polynomial only.
9	Divide by wavelength	No equivalent (May be done manually by Compute)	
11	Correct for reference changes	No equivalent	Performed by instrument ⇒ Information just copied from data to model file.
13	Full MSC	Smoothing, Moving average + MSC, Full	Vision only.
31	Savitsky&Golay 1st derivative	S. Golay Derivation, 1st order	2nd order polynomial only. Vision only.
32	Savitsky&Golay 2nd derivative	S. Golay Derivation, 2nd order	As above.
	No equivalent	Normalization	

The abbreviations used in the Unscrambler log files are explained in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

File - Export Model - Vision ...

With this option you can export a result file to Vision format. This model can then be imported into the software package controlling your instrument. All necessary parameters for export to Vision are not always found in the data and/or model files and must be entered by you. This is explained in more detail in the Chapter NSAS Transformations.

The **Vision Export** dialog is more or less similar to the **NSAS Export** dialog. It contains the three sheets General, Instrument Parameters and Math.

Vision Export Dialog: General and Instrument Parameters Sheets

These sheets are identical to the sheets in the **NSAS Export** dialog (see File - Export Model - NSAS ...).

Vision Export Dialog: Math Sheet

This page of the property sheet is used to specify which transformations have been applied to the data before calibration has been performed. This is important for use of the exported model for predictions, as spectra used as input to the prediction must undergo exactly the same transformations as the calibration spectra.

Vision allows for up to three transformations, specified in the fields 1st NSAS transformation, 2nd NSAS transformation and 3rd NSAS transformation respectively.

The first transformation is used for the sole purpose of indicating whether the spectra has been corrected for reference changes within the instrument or not.

The second and third transformations may be any Vision math type, including None. Select from the drop-down list. For some of the math types, one or more of the parameters Segment size, Gap size, or Divisor point will be enabled. These will be written to the model file exactly as shown. Use the spin buttons to specify them.

Default values for the transformations are taken from the Instrument Information block in The Unscrambler's result file, which is again copied from The Unscrambler's data file. If the data file was originally imported from an NSAS data file, the Instrument Information block was created based on the information found in the NSAS data file, reflecting any transformations applied to the data before the NSAS data file was created. For this reason, you should not change any default values unless you are very confident in what you are doing.

Any transformation applied to the raw data using The Unscrambler must be manually specified. For more information about the correspondence between Unscrambler and NSAS transformations, see the Chapter NSAS Transformations.

Press the Log button on this sheet to enter a Log where you can make notes about your export.

File - Export Model - Tracker ...

Tracker models are written in a format used by Foss' instruments. You can write models in both .CAL and .PIF format.

Specify the folder in which you want to save the model in the Folder field in the **Export Tracker Model** dialog. Use the Browse button if you do not remember the folder name. Then, in the Model name field, enter the name you want the model file to have on the disk.

In the PCs field, enter the number of PCs you want the model to be made up of in the exported model file. This will usually be the optimal number of components you have found during your work in The Unscrambler.

There are two types of Tracker models; CAL and PIF.

File - Convert Vector to Data Table

The menu option **File - Convert Vector to Data Table** allows you to convert a row or a column of a data table (2-D or 3-D) into a two-way data table. This feature is particularly useful when the selected vector is one of the following:

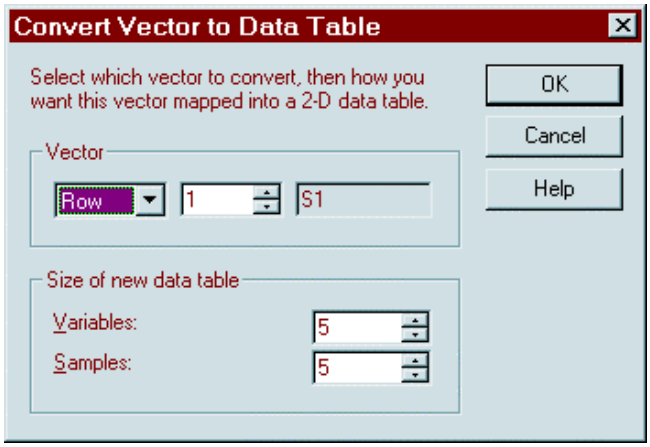
- Column of 3-D data table with layout O^2V.
- Row of 3-D data table with layout OV^2.
- Column of a data table containing unfolded three-way data with several blocks below each other.
- Row of a data table containing unfolded three-way data with several blocks side by side.

Once the vector has been converted into a 2-D data table, you may perform operations which were not possible with a 3-D layout.

Note: Only one vector at a time can be converted.

The figure below shows the **Convert Vector to Data Table** dialog.

Dialog: Convert Vector to Data Table



In the **Vector** section, choose an orientation (Row / Column) and select the desired vector.

In the **Size of new data table** section, tune the numbers of Variables and Samples.

Click **OK** to display the new table.

File - Duplicate

You can duplicate designed data tables in The Unscrambler. There are 4 options under **File - Duplicate**:

- Duplicate as Non-design
- Duplicate as Modified design
- Duplicate as 2-D data table
- Duplicate as 3-D data table

File - Duplicate - As Non-design

The designed data table is copied to a normal data table in a new Editor. All design information is lost in the process, and the data is not locked anymore. This means that you can modify the data with transformations and computations.

File - Duplicate - As Modified Design

The current designed data table is used as a basis for creating a new design. The **Design Wizard** is launched from the dialog **Define Design Variables** (see p. 104) with all settings of the current design. It is then easy to go through the steps and make minor changes to the design, instead of starting from scratch to make a new design that is similar.

File - Duplicate - As 2-D Data Table

The menu option **File - Duplicate - As 2-D Data Table** allows you to convert a three-way data table into a two-way data table.

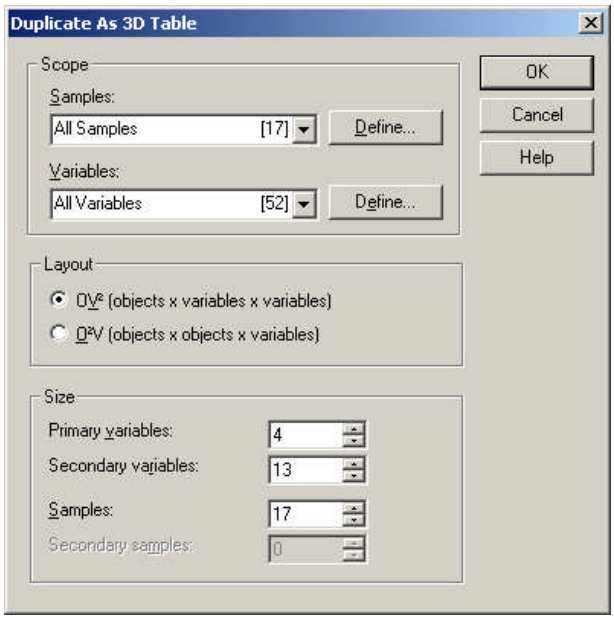
This feature is useful when you want to run an analysis meant for two-way data (e.g. PCA or PLS).

File - Duplicate - As 3-D Data Table

The menu option **File - Duplicate - As 3-D Data Table** allows you to convert a two-way data table into a three-way data table.

This feature is useful when you already have a two-way data table containing your unfolded three-way data. It creates a new 3-D table with the appropriate three-way layout (OV^2 or O^2V) and reorganizes your data accordingly.

Dialog: Duplicate as 3D Table



In the **Duplicate as 3D Table** dialog, specify the scope (samples and variables) of the data to be converted to 3-D layout.

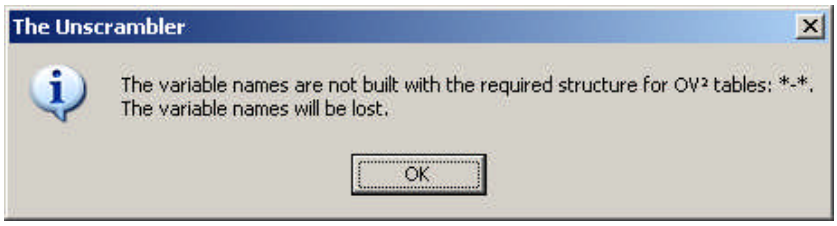
In the layout field, select either OV^2 or O^2V.

Finally, define the size of the blocks of variables / samples:

- If the layout is OV^2, type in the number of Primary and Secondary variables.
- If the layout is O^2V, type in the number of Primary and Secondary samples.

Click OK when your 3-D table is fully specified.

Note: If the original data table contains variable names (or sample names for O^2V) with a "*-*" structure (e.g. Gum-1, Gum-2, …, Gum-6, Adh-1, Adh-2 etc.), the names will be kept in the new 3-D table. Otherwise a warning is displayed:


The Unscrambler
The variable names are not built with the required structure for OV² tables: *-*.
The variable names will be lost.
OK

File - Print Lab Report…

You can print a form which the laboratory can use when they perform the experiments, e.g. to write down the response values. You see common information like sample names, who created the design at which time, etc., in addition to the laboratory report outline.

This option is only available when a design file is marked in the file dialog.

Initially, you enter the dialog **Print Lab Report**. If you want to include your own notes in the print-out, select the Notes check button. If you want to change the page setup, select the Setup button, which brings you to the **Print Setup** dialog. When you are satisfied with your choices, click OK.

File - Print…

or **Ctrl+P**

You enter the **Print** dialog, which lets you control how you transfer the current document to a printer or file.

You may print either Current plot, or All Plots. Select Current Plot if you wish to print out only the currently active plot on screen; select All Plots if you whish to print out all plots currently shown on screen.

In the field Print range you decide what to print by selecting the appropriate radio button. The print range applies to the current window in the Workspace. Use Selection if you have selected a range in the current window which you want to print.

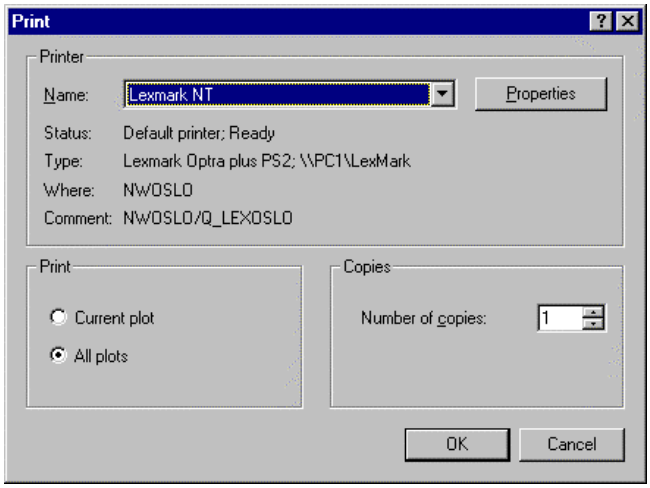
Finally, use the spin button to select how many copies of your document you want to print.

Note: You need to have a file open (in the Editor or the Viewer) to have access to this option.

Printing out Several Plots

The **Print** dialog for plots offers the possibility to print either Current plot, or All Plots. Select Current Plot if you wish to print out only the currently active plot on screen; select All Plots if you wish to print out all plots currently shown on screen.

The Print dialog for plots



Select the printer you want to use from the drop-down printer list. The properties of the printer can be viewed by pressing Properties. See your Windows documentation or printer manual for information on setting up your printer. You can print to a file by clicking on the Print to file box.

File - Print Preview

It is a good idea to preview a document before sending it to the printer. Print preview lets you take a look at how your pages will look when they have been printed. The option is only available if a file is currently open.

File - Print Setup…

In the top field of this dialog, Printer, you specify which printer to use for your print-out. Press the Properties button to enter a dialog where you may specify details about the print-out, such as orientation, multipage printing, etc..

In the Paper field, you specify the size of the paper and the paper source if necessary. Finally, specify whether to print out as portrait or landscape by selecting the appropriate radio button in the Orientation field.

File - Lock

This command disables all changes to the contents of a data table.

Locking data sets is a recommendation of the 21 CFR Part 11 guidelines from the FDA.

Once a file is locked, the usual Editor operations performed with the Edit and Modify menus (copy, paste, replace, transform etc…) are disabled, as well as direct data input and import of new data. In the General sheet of the **Properties** dialog, the file is shown as "Read Only" and the Summary field at the bottom mentions "This file is currently locked".

Note: Locking a file does not prevent you from running analyses on the data. Those analyses will automatically be kept track of in the Log sheet of the **Properties** dialog as usual.

To enable changes in the data table, use **Feil! Fant ikke referansekilden.** as described hereafter.

File - Unlock

This command enables changes to the contents of a data table that was previously locked (see **Feil! Fant ikke referansekilden.** above).

In the General sheet of the **Properties** dialog, the file is shown as "Read / Write" and the Summary field at the bottom mentions "This file is currently unlocked".

File - Properties…

Information about the contents of the data or result file in the current window is shown in the **Properties** dialog. The shortcut button (see above) on the Toolbar takes you directly to the Notes sheet of the dialog.

The **Properties** dialog contains up to 5 out of a total of 7 available sheets which have the following names:

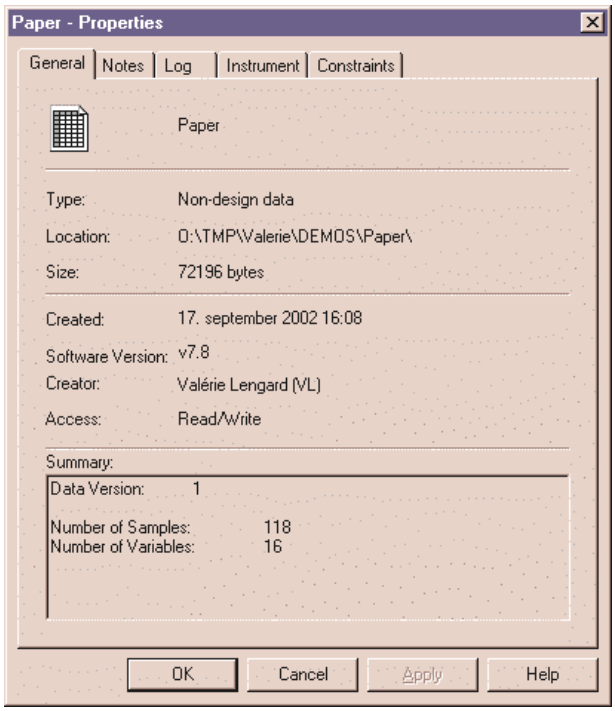
- General
- Notes
- Log
- Instrument
- Transformations
- Model
- Constraints

All sheets are not displayed for every file.

Properties Dialog: General Sheet

This sheet displays general information on the current Unscrambler file, such as the type of data, location, and size of the file. You will also see who created the file and at which date, as well as a short summary of the contents of the file.

Dialog: Properties - General Sheet



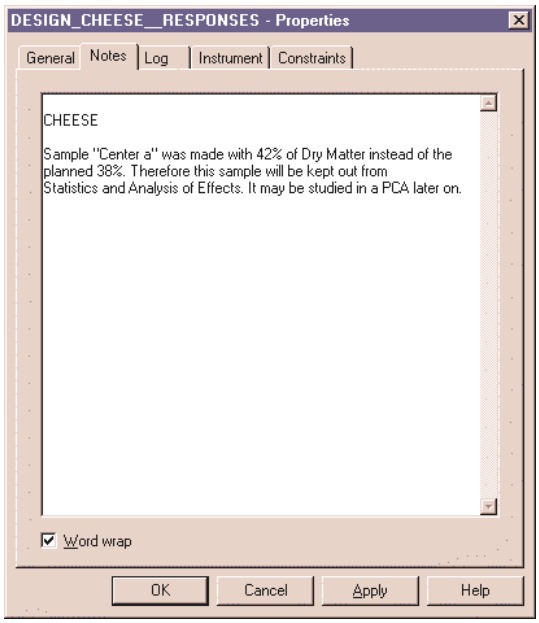
Properties Dialog: Notes Sheet

This sheet is where you can add comments about the data or results stored in a file, their purpose, the analyses you are doing etc.

The notes you type in follow the data file. They are also copied to all result files based on the data table, if you have selected this option in **System Setup**.

You do not need to enter notes regarding editing and transformations done from the menus in The Unscrambler, since this is automatically written to the Log sheet.

Dialog: Properties - Notes Sheet


DESIGN_CHEESE__RESPONSES - Properties
General
Notes
Log
Instrument
Constraints
CHEESE
Sample "Center a" was made with 42% of Dry Matter instead of the planned 38%. Therefore this sample will be kept out from Statistics and Analysis of Effects. It may be studied in a PCA later on.
Word wrap
OK
Cancel
Apply
Help

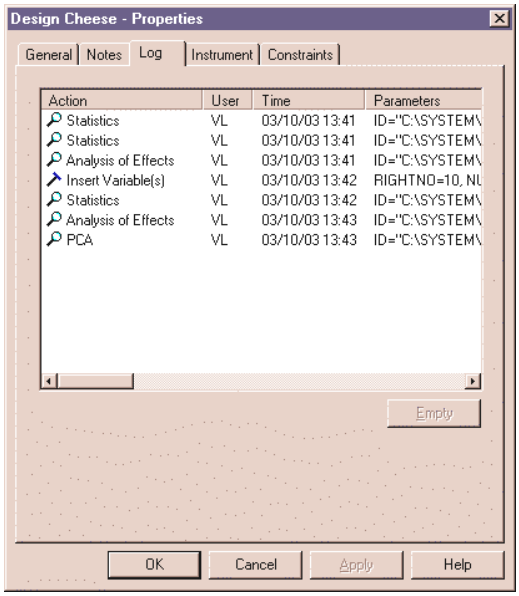
Properties Dialog: Log Sheet and Transformations Sheet

This sheet is called “Log” for data files, and “transformations” for result files.

Data Table

A Log of all transformations and other changes to the data table is displayed in this sheet.

Dialog: Properties - Log Sheet



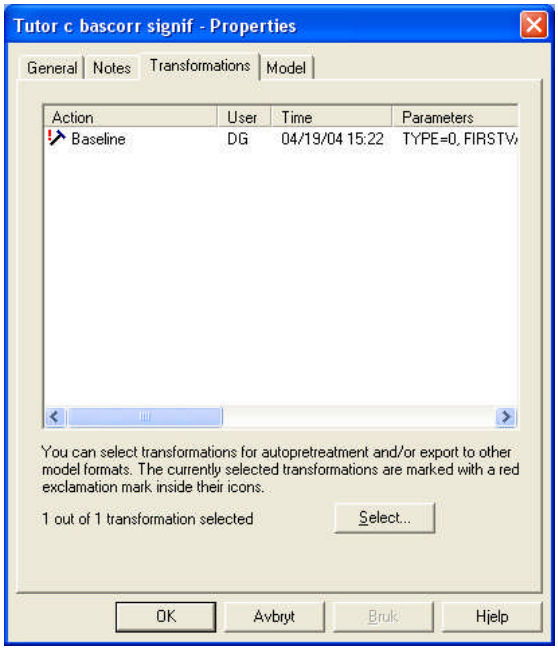
The Empty button is used to erase all Log records for the current data file. This button is disabled if the Supervisor has not authorized the option for the current user. Enability/disability of the Empty button is set in the Supervisor **System Setup** options.

In the Parameters column, abbreviations are used to tell which transformations have been done. See the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices , for details about the abbreviations used in The Unscrambler.

Result File

Only the transformations performed on the data table are displayed in the Transformations sheet. These transformations are the same as recorded in the Log for data files.

Dialog: Properties - Transformations Sheet

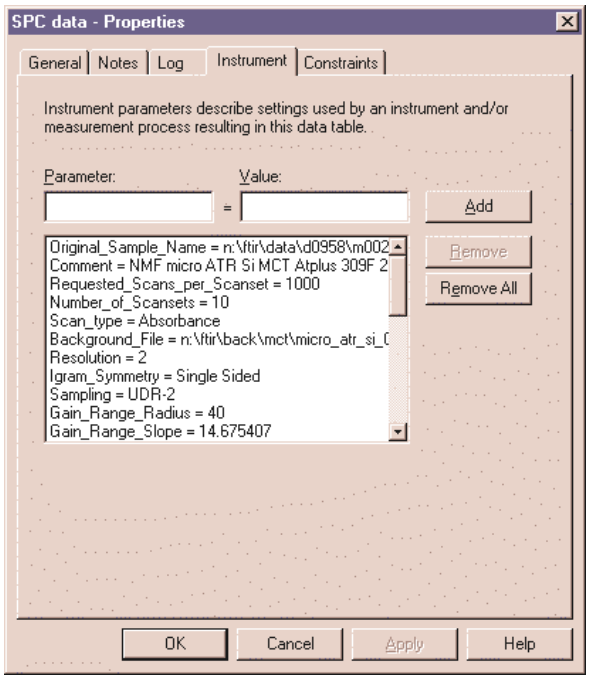


At the bottom of the sheet, a Select button allows you to select the transformations that you wish to apply to new data as ***automatic pre-treatments*** upon using the model at a prediction or classification stage. Clicking the Select button opens the Select Transformations dialog (see p. 90).

Properties Dialog: Instrument Sheet

This sheet exists only for data files. When data are imported from e.g. NSAS and JCAMP, there are some parameters which do not fit into the Unscrambler data format. These parameters are stored in the Instrument sheet and are used for file export at a later stage. This is only possible for the data tables, and not for results, so if you need instrument parameters when you export a model, set these parameter in the data file, then perform the calculation and the export of the model.

Dialog: Properties - Instrument Sheet

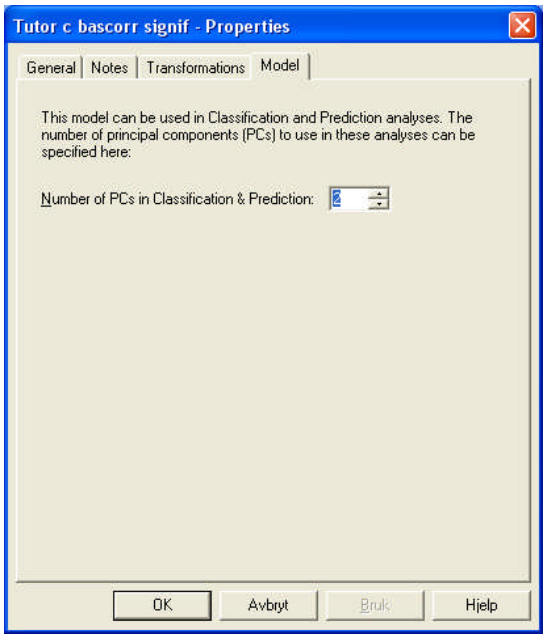


You may enter your own instrument parameters, if additional information is needed. The instrument parameters are explained in more detail in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

Properties Dialog: Model Sheet

The Model sheet is only available for result files. This is where you set the number of components you want used as default when the model is used for prediction or classification. This is necessary if the number of components you want to use is different from the optimal number of components suggested by The Unscrambler. You can override this default in the prediction and classification dialog.

Dialog: Properties - Model Sheet

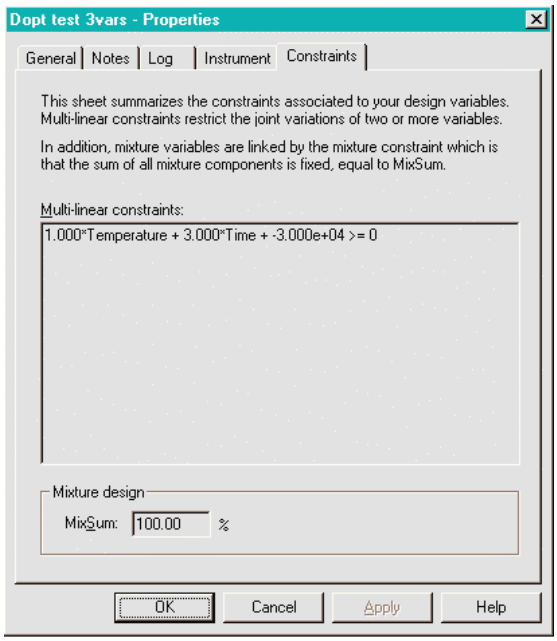


Properties Dialog: Constraints Sheet

This sheet only applies to data tables. In this page, find a summary of the settings for your D-Optimal or Mixture design:

- Recapitulation of the multi-linear constraints
- MixSum value
- For non-designed tables with mixture variables, the MixSum value can be changed in this page. Values which do not respect the lower and upper bounds of your mixture variables will be rejected.

Dialog: Data Table Properties - The Constraints Sheet



Select Transformations Dialog

This dialog is accessed from the Pretreat button in the **Classification** or **Prediction** dialog, as well as the Select button in the Transformations sheet of the **Properties** dialog.

It allows you to select the transformations that you wish to apply to the data as automatic pre-treatments upon classification or prediction.

You may select among the available transformations either manually or with the help of the Select All button.

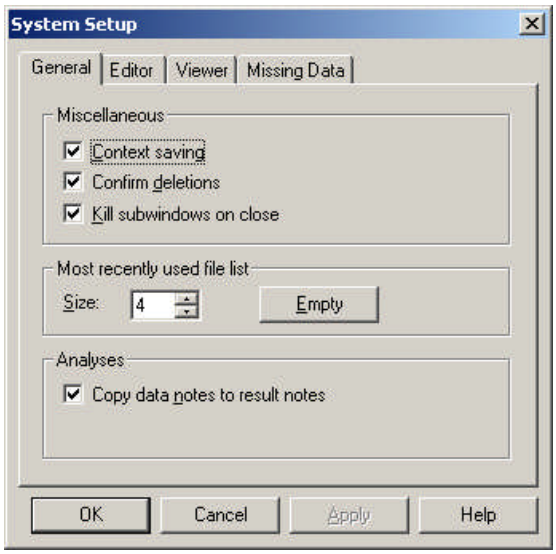
Clicking Select None tells the system not to use any of the transformations.

Your choice is validated once you click OK.

File - System Setup…

This option lets you enter the **System Setup** dialog as seen in the figure below, where you can configure The Unscrambler to suit your own preferences when you work. Any changes you make will affect only your own user account and all files you work on. Pressing Apply brings the changes into immediate effect. The action cannot be canceled.

Dialog: System Setup



The dialog contains four sheets: General, Editor, Viewer and Missing Data.

Note: If you have logged in as ***Supervisor***, the System Setup dialog is different from the current description; lookup Chapter System Configuration in Practice for more information.

System Setup Dialog: General Sheet

The options in this sheet rule the general use of The Unscrambler in connection to your user account.

In the **Miscellaneous** field you can tick one or more of the three available tick-boxes:

- If you tick the box Context Saving, The Unscrambler saves the entire workspace when you exit. All Editor and Viewer documents will be opened again the next time you open The Unscrambler;
- The box Confirm deletions ensures that The Unscrambler asks you for confirmation before deleting any samples, variables, etc.;
- An Editor or Viewer window may have other windows derived from themselves, for example a Sample Statistics Editor opened as a sub-window. Select the option Kill subwindows on close if you want all sub-windows to close automatically when you close the parent window.

In the field **Most recently used file list** you can define how many of the projects you have previously worked on are to appear on the list at the bottom of the **File** menu. Use the Empty button to remove all current entries in the file list. This may be appropriate if you have files in the list that reside on other PCs in the network, as this may slow the performance down.

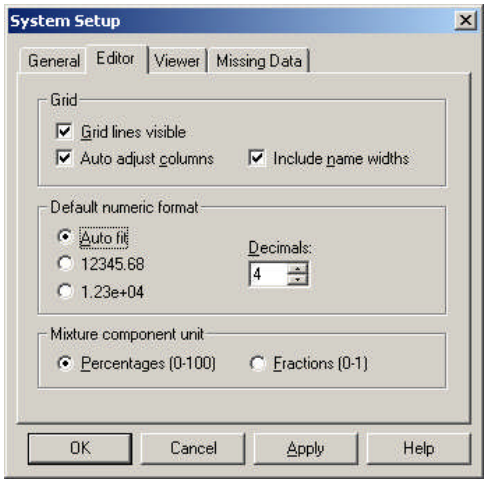
In the last field, **Analysis**, you may tick one or both of two available tick-boxes:

- The tick-box Copy data notes to result notes lets you automatically copy all the notes which you take at any stage of your analysis to all result files you create from models derived from the data table. The notes are originally stored in a file which follows your data table;
- The box Reduce result file size (no residuals) lets you select not to save all matrices in a result file when you close the file. The matrices which are not stored are: Eix; Fiy; xWeighted; yWeighted. This means that before you save the file for the first time, or before you close it, you can view all types of plots, but once you have done this, you can only view plots which do not contain any of the matrices not saved.

System Setup Dialog: Editor Sheet

The options provided on this sheet apply only to the Editor Stage.

Dialog: System Setup - The Editor Sheet



In the field **Grid** three tick-boxes are available:

- You can turn grid lines on or off by selecting or deselecting the box Grid Lines Visible;
- The box Auto adjust columns makes The Unscrambler automatically change the width of the columns in the Editor to give enough room for your data. Column widths are by default adjusted to fit only the numbers, not the variable names;
- If you tick the box Auto adjust columns, you can also choose to adjust the column width to show both numbers and names in full by ticking the last box, Include name widths.

In the field **Default numeric format** you select the default format of the data values. There are three possibilities, as shown below:

Default format of data values

Option	Description
Autofit	The system decides the format
“12345.6789”	Normal layout
“1.2345e+04”	Scientific notation

Use the Decimals spin button to define how many decimal places to use in the latter two options. Scientific format allows a minimum of four decimals and normal layout allows a number without decimals.

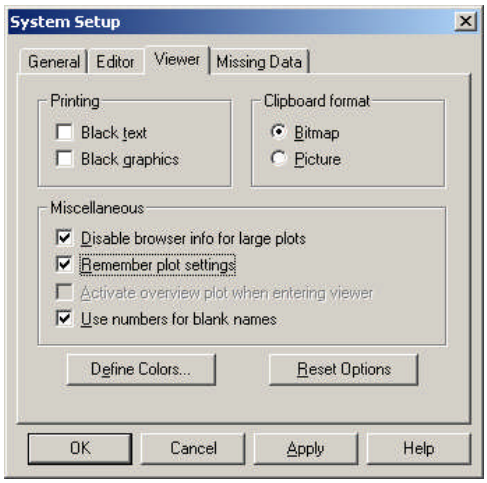
Note: The Unscrambler uses the IEEE 754 standard data format. Numbers are stored with six or seven significant digits. If you select several decimal places, and more than seven digits are shown in the Editor, you should be aware that the last digits may be noise. We recommend that you use the Autofit option to avoid this.

Use the **Mixture component unit** field to denote mixture components either as percentages (0-100%) or as fractions (0-1). The default is to use percentages.

System Setup Dialog: Viewer Sheet

The appearance of the Viewer Stage and the plotting speed are affected by the properties in this sheet.

Dialog: System Setup - The Viewer Sheet



The quality of the plot may be poor if you print a plot full of colors on a non-color printer. This is due to how the colors are mapped in the printer. Tick the boxes Black text and/or Black graphics in the **Printing** field if you want the text and/or graphics to be plotted using black instead of gray tones.

Plots can be inserted into other programs either as a Bitmap or as a meta file (Picture). You can choose one of those options in the **Clipboard format** field. If the plot has many objects (many samples and/or variables, using symbols layout, etc.), it will occupy less space in the other programs if you choose the Bitmap option. For plots with few objects, it may be the other way around.

In the **Miscellaneous** field you have 4 choices:

- Large data matrices (more than 5000 elements) may be slow to plot. By checking the box Disable browser info for large plots, the plotting time is reduced. The disadvantage is that you can no longer click at a data point to get information regarding that point.
- By checking the box Remember plot settings, you enable easy customization of the result plots you want to display when opening a previously saved results file. The plots appearing in the Viewer when you open a model file will be the same ones that were on screen the last time you saved the model. Un-check this box to disable customization.
- Check the box Activate overview plot when entering viewer if you want the overview plots to appear when you click View in the progress dialog after an analysis. If this choice is not selected, the Viewer will be empty and you have to select a plot from the **Plot** menu, unless you have checked the previous box (Remember plot settings), in which case the current choice is grayed out.
- Markers/labels that are blank or contain a star are replaced by the sample/variable number in plots when the option Use numbers for blank names is selected. Uncheck it to display the data point without the number.

Viewer Colors

If you click the button Define Colors on the Viewer sheet, you enter the dialog **Viewer Colors**, where you can change the default colors of all elements in the plots to suit your needs for documentation.

In the field Device you can set up different colors for use on screen and for output on printer.

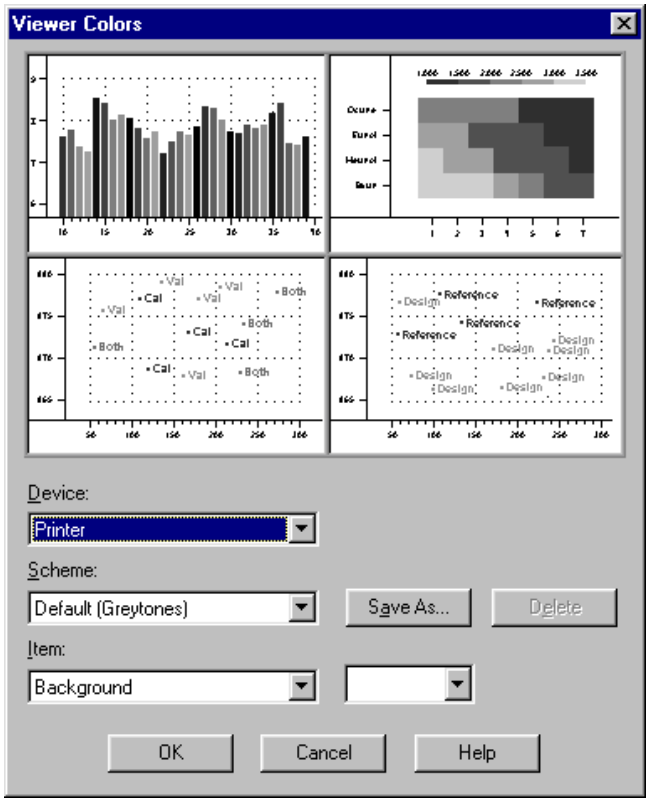
Default colors can be restored by selecting 1 of the 2 predefined schemes from the drop-down menu in the Scheme field. There is one with white and one with black background.

In the Item field you can select the plot item you want to change the color for and set the color using the box to the right of this menu box.

Color Scheme for Black and White Printing

In the Viewer, The Unscrambler uses colors that make it easy to distinguish different curves or other objects on screen. However, when printing out plots on a black & white printer these colors sometimes appear very similar. In such a case, a new default color scheme can be used. From the **Viewer Colors** dialog, shown below, select the following options: Device: printer; Scheme: Default (Greytones).

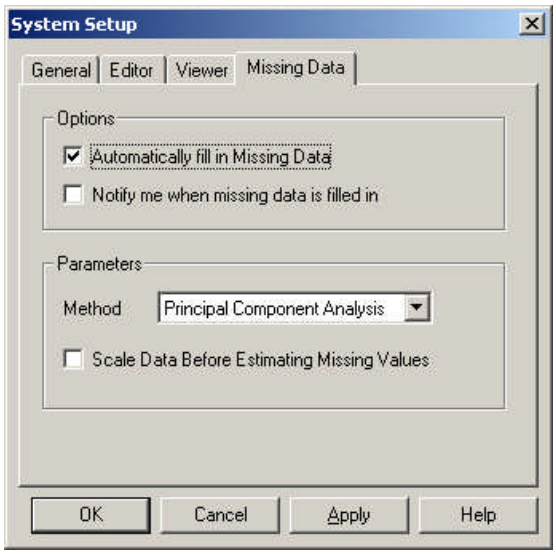
The Viewer Colors dialog offers a "Greytones" defaults setting



System Setup Dialog: Missing Data Sheet

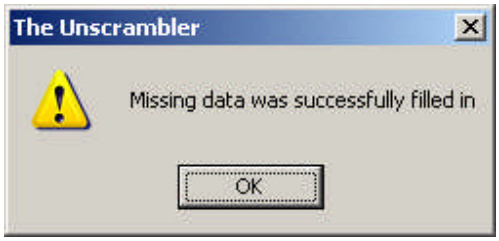
The options provided on this sheet will apply to all data tables you open in the Editor.

Dialog: System Setup - The Missing Data Sheet



In the Options frame, choose whether you want to Automatically fill in Missing Data. When this option is checked, any new table with some missing data opened in the Editor will have all its missing values filled in with estimated values prior to being displayed on screen.

If you also select Notify me when missing data is filled in, a small information dialog will appear every time this happens, as shown below:



In the Parameters frame, choose the estimation Method: Principal Component Analysis or Row Column Mean Analysis.

You may optionally Scale Data Before Estimating Missing Values by ticking the box at the bottom. This is recommended if the variables you usually deal with are measured in different units or have different scales.

For more details on specific cases of tables with missing data, lookup chapter Fill Missing - Difficult Situations p. 121.

File - Recent Files List

The list of recently opened files is displayed at the bottom of the **File** menu list, just above the last menu option "**Exit**". The most recently opened file is listed first, then the second most recent and so on. The file type is displayed to the right of the file name, as either [d] (data table) or [r] (result file).

To re-open a file from the list, click on the desired file name, or press <Alt> + <F> and type the corresponding number.

Note: The option is disabled if you are logged in as supervisor.

By default, the list contains up to 4 files. You may change that number in the General sheet of the **System Setup** dialog, as described p.91.

File - Exit

Through this option you can quit The Unscrambler. You are prompted to save any data files that have changed since the last time they were saved.

The Design Wizard

File - New Design

Use this option if you wish to create a new design, or to modify or extend an existing design.

The Design Wizard

The Design Wizard can be accessed through two different commands.

If you chose **File - New Design**, the first dialog is **Select Method to Use**, where you will have to choose between starting from scratch, modifying or extending an existing design.

If you chose **File - Duplicate - As Modified Design**, the first dialog is **Define Design Variables**, where you may add new design variables, modify the properties of existing ones or remove them.

Design Wizard Dialogs

The Design Wizard contains a dynamic sequence of dialogs, where the type of dialog coming next often depends on your choices in the current dialog.

The best way to get help on a specific dialog is to click the Help button when using that dialog in The Unscrambler.

However, if you wish, you may lookup each individual dialog by selecting it from the list hereafter.

Alphabetical list of Design Wizard dialogs

Dialog name	Description on page…
Design Wizard - Define Design Purpose	p. 112
Design Wizard - Define Design Variables	p. 104
Design Wizard - Define Mixture Variables	p. 107
Design Wizard - Define Model	p. 111
Design Wizard - Define Non-design Variables	p. 107
Design Wizard - Define Process Variables	p. 109
Design Wizard - Design Details	p. 116
Design Wizard - Design Type	p. 116
Design Wizard - Design Type (Mixture)	p. 112
Design Wizard - Enter Multi-Linear Constraints	p. 109
Design Wizard - Extend a Central Composite Design	p. 102
Design Wizard - Extend a Centroid Design	p. 103
Design Wizard - Extend a D-optimal Mixture Design	p. 102
Design Wizard - Extend a D-optimal Non-mixture Design	p. 102
Design Wizard - Extend a Fractional Factorial Design	p. 101
Design Wizard - Extend a Full Factorial Design	p. 100
Design Wizard - Extend a Lattice Design	p. 102
Design Wizard - Extend an Axial Design	p. 103

Design Wizard - Generate Design	p. 113
Design Wizard - Last Checks	p. 118
Design Wizard - Randomization Details (General)	p. 117
Design Wizard - Select Design Type	p. 98
Design Wizard - Select Existing Design	p. 100
Design Wizard - Select Method To Use	p. 98

Design Wizard - Select Method To Use

This is where you can choose between starting from scratch, modifying or extending an existing design by selecting the appropriate radio button. Read the contents of the Information field at the bottom, to get more details about the currently selected option.

Once you have made your choice, click Next to access the next dialog.

Note: Use Modify Existing Design only if the new design you want to create through the modification is of the same type as the existing one.

Select Method To Use - Next Dialog

- If you have selected From scratch, you access the dialog **Select Design Type**.
- If you have selected Modify existing design or Extend existing design , you access the dialog **Select Existing Design**.

Design Wizard - Select Design Type

This dialog is accessed when you have chosen to build a design "from scratch". This is where you can build a completely new design.

In the **Select Design Type** dialog you can choose between three types of classical screening designs, two types of classical optimization designs, and two additional types of design, by selecting the appropriate radio button and clicking Next.

Different Types of Experimental Design

The designs with their fields of application and the allowed number of design variables are listed below.

Available types of experimental design

Type of Design	Field of Use	Allowed number of design variables
Full Factorial Design	**Screening Design** a) You have few design variables (2 to 6) and want to study all main and interaction effects independently from each other. b) One of your design variables has more than 2 levels.	2 - 6
Fractional Factorial Design	**Screening Design** Most useful in the early stages of a research project, when the number of design variables may be large and the goal is to find	3 - 15

	out with a small number of experiments which variables should be investigated further. **Note!** This design only allows 2 levels for each design variable.	
Plackett-Burman Design	**Screening Design** An alternative to fractional factorial designs, in the early stages where you study main effects only. The number of experiments is minimized: never more than number of design variables + 4. **Note!** This design only allows 2 levels for each design variable.	4 - 32
Central Composite Design	**Optimization Design** Finds the optimal settings of your design variables by adding a few more experiments to a full factorial design. **Note!** All design variables must vary continuously between a low and a high level.	2 - 6
Box-Behnken Design	**Optimization Design** An alternative to central composite designs, when you have reason to believe that the optimum of your response is not in the corners of the experimental region, and if you are not interested in extending a previous factorial design. **Note!** All design variables must vary continuously between a low and a high level.	3 - 6
D-Optimal Non-mixture Design	You have only Process variables, and some of these present Multi-Linear Constraints **- Screening** **- Optimization**	 2-12 2-6
Mixture Design	You have Mixture variables, and possibly some Process variables in addition. Some of the Mixture or some of the Process variables can be constrained. **- Screening** **- Optimization** According to your specifications, one of 4 designs can be used : - Simplex-Lattice Design - Simplex-Centroid Design - Axial Design - D-Optimal Mixture Design[1]	 3-15 or 32 (Axial) 3-6

1- A D-Optimal Design will be used with Mixture variables if the experimental region is not a simplex, in particular if some of your mixture variables present Multi-Linear constraints.

Select Design Type - Next Dialog

It is easy to set up a design from scratch in The Unscrambler: Once you have made your choice in the **Select Design Type** dialog and clicked Next, you will enter a string of dialogs which tell you exactly what to do. Simply fill in the necessary information in each dialog and press Next. If you make a mistake, you can always go back to a previous dialog by pressing Back.

According to the type of design you have selected, the next dialog will be as follows:

- Full Factorial, Fractional Factorial, Plackett-Burman, Central Composite or Box-Behnken: **Define Design Variables**
- D-optimal Non-mixture: **Define Process Variables**
- Mixture: **Define Mixture Variables**

Design Wizard - Select Existing Design

This dialog lets you re-use the specifications of an existing design.

If you remember the name of the file you want to re-use, you can enter it directly; if not, you can click Browse to enter one of the two dialogs **Select Design to Modify** or **Select Design to Extend** (see below for details), where you can look for the appropriate file.

Select Design to Modify

This dialog is accessed by pressing the Browse button in the **Select Existing Design** dialog, and is identical to the **Open File** dialog. Select the data file you wish to modify and press Open.

Select Design to Extend

This dialog is accessed by pressing the Browse button in the **Select Existing Design** dialog, and is identical to the **Open File** dialog. Select the data file you wish to extend and press Open.

Select Existing Design (Modify) - Next Dialog

According to the type of design you have selected, the next dialog will be as follows:

- Full Factorial, Fractional Factorial, Plackett-Burman, Central Composite or Box-Behnken: **Define Design Variables**
- D-optimal Non-mixture: **Define Process Variables**
- Mixture: **Define Mixture Variables**

Select Existing Design (Extend) - Next Dialog

Once you have chosen the design you want to extend and clicked Next, you enter a dialog called **Extend a (X) design** (where (X) represents the type of design in question), where all available extension options are listed.

Note1: Variables are shown in red if they are incompatible with the type of design extension that you have chosen. If this happens, select another extension or change the properties of the variable to fit the extension you want to do.

Note2: Box-Behnken and Plackett-Burman designs cannot be extended.

Note3: If any Design point is changed in a D-Optimal or a Mixture design data table, the design can no longer be extended. This does not apply to changes in Reference samples.

Design Wizard - Extend a Full Factorial Design

This dialog gives you 3 choices regarding the extension of a full factorial design.

Delete Design Variables and Add More Levels

More levels are typically added to a category variable when you find that some levels are missing. Mark levels you want to keep out of the design and click the button between the two lists to remove them.

You enter the following dialogs: **Define Design Variables**, **Define Non-design Variables**, **Design Details**, **Randomization Details**, **Last Checks**.

Add Center and Reference Samples or Replicates

Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare.

You enter the following dialogs: **Design Details**, **Randomization Details**, **Last Checks**.

Extend to Central Composite Design

Use the central composite design when you go from the screening phase to the optimization phase.

You enter the following dialogs: **Define Design Variables**, **Define Non-design Variables**, **Design Details**, **Randomization Details**, **Last Checks**.

Note: Category variables must be removed before the design is extended to a central composite design.

Design Wizard - Extend a Fractional Factorial Design

In this dialog, you have the choice between the following 4 extensions

Delete Design Variables

Design variables that are found to be insignificant can be removed from the data table before you go on with further analyses.

You enter the following dialogs: **Define Design Variables**, **Define Non-design Variables**, **Design Type**, **Design Details**, **Randomization Details**, **Last Checks**.

Add Center and Reference Samples or Replicates

Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare.

You enter the following dialogs: **Design Details**, **Randomization Details**, **Last Checks**.

Extend to Full Factorial Design

Full factorial designs are useful when you need to examine all interactions and can afford to do all the experiments.

You enter the following dialogs: **Define Design Variables**, **Define Non-design Variables**, **Design Details**, **Randomization Details**, **Last Checks**.

Extend to Central Composite Design

Use the central composite design when you go from the screening phase to the optimization phase.

You enter the following dialogs: **Define Design Variables**, **Define Non-design Variables**, **Design Details**, **Randomization Details**, **Last Checks**.

Note: Category variables must be removed before the design is extended to a central composite design.

Design Wizard - Extend a Central Composite Design

The only extension option for Central Composite Designs is to add center and/or reference samples and replicates. Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare to them.

You enter the following dialogs: **Design Details**, **Randomization Details**, **Last Checks**.

Design Wizard - Extend a D-optimal Non-mixture Design

You can extend a D-Optimal Non-mixture Design by adding reference samples, center points or replicates.

Tick the radio button Add Center and Reference Samples or Replicates and press Next.

You will enter the following dialogs: **Design Details** and **Last Checks**.

Design Wizard - Extend a D-optimal Mixture Design

You can extend a D-Optimal Mixture Design by adding reference samples, center points or replicates.

Tick the radio button Add Center and Reference Samples or Replicates and press Next.

You will enter the next dialog: **Design Details**.

Design Wizard - Extend a Lattice Design

In this dialog, you have the choice between the following 4 extensions.

Add Levels on Category Process Variables

This radio button is only available if you defined Category Process variables in your first design.

The next dialog will be: **Define Process Variables**.

Add Center and Reference Samples or Replicates

Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare.

The next dialog will be: **Design Details**.

Increase Lattice Degree

A Lattice design can be extended from degree 1 to 2-5, or from degree 2 to 4.

The next dialog will be: **Design Type (Mixture)** where you can set the desired degree.

Note: Increasing the Lattice degree is only possible if your first design has a degree of 1 or 2. Higher-degree lattices can only be extended to Centroid.

Extend to Centroid Design

This choice first leads you through dialogs **Define Non-design Variables** and **Define Model**. Then you enter the dialog **Design Type (Mixture)** where the recommended extension design is: Centroid Design with Interior Points. Select this design and click Next.

The next dialog will be: **Design Details**.

Note: It is not possible to create a Centroid design if you have more than 6 mixture variables.

Design Wizard - Extend a Centroid Design

In this dialog, you have the choice between the following 2 extensions.

Add Center and Reference Samples or Replicates

Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare.

The next dialog will be: **Design Details**.

Add Interior Points

If they are not already included in your Centroid design, you can choose to add Interior Points.

The next dialog will be: **Design Details**.

Design Wizard - Extend an Axial Design

In this dialog, you have the choice between the following 3 extensions.

Add Center and Reference Samples or Replicates

Center samples and replicates are added to increase the reliability of the model. Add reference samples to see how your design samples compare.

The next dialog will be: **Design Details**.

Add End Points

If they are not already included in your Axial design, you can choose to add End Points.

The next dialog will be: **Design Details**.

Extend to Centroid Design

This choice first leads you through dialogs **Define Non-design Variables** and **Define Model**. Then you enter the dialog **Design Type (Mixture)** where the recommended extension design is: Centroid Design with Interior Points. Select this design and click Next.

The next dialog will be: **Design Details**.

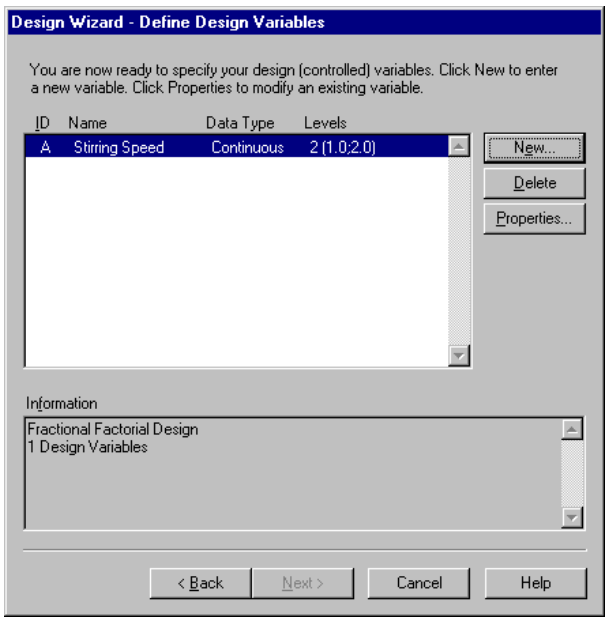
Note1: You cannot extend a 3-variable Axial design with End Points to a 3-variable Centroid Design with Interior points, these two designs are strictly identical!

Note2: It is not possible to create a Centroid design if you have more than 6 mixture variables.

Design Wizard - Define Design Variables

In this dialog, you specify the design variables that you need to have in your new design.

Dialog: Define Design Variables



The top field displays information about all defined design variables, while the Information field displays information about the currently selected variables and design.

The dialog allows you to add a new or to delete or change an already defined variable by clicking one of the buttons New, Delete or Properties. Clicking New or Properties leads you to the **Add Design Variable** (or **Variable Properties**) dialog where you can specify the name and properties of the design variable.

For Central Composite designs, this dialog also includes an extra field star points distance from center, in which you may tune the distance between star points and design center. Access to this field is allowed once you have defined at least two design variables.

Define Design Variables - Next Dialog

Once you have added all necessary design variables by clicking New or changed their definitions by clicking Properties, you may proceed by clicking Next. You will then access the next dialog **Define Non-design Variables**.

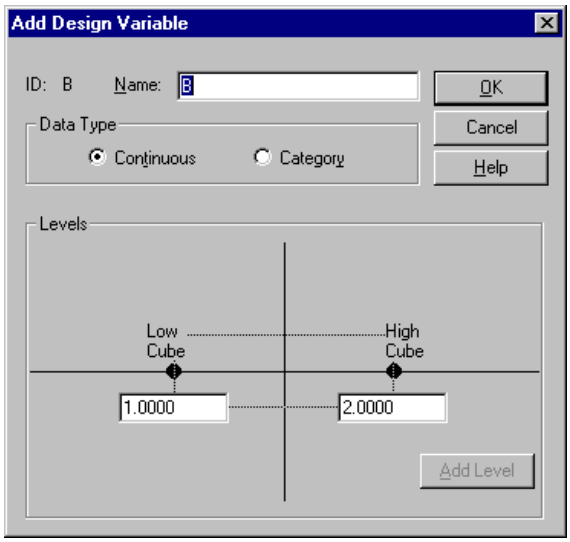
Add Design Variable / Variable Properties Dialog

When you select respectively New or Properties in **the Define Design Variables**, the **Define Mixture Variables** or the **Define Process Variables** dialog you enter a dialog called **Add Design Variable** or **Variable Properties** respectively. In this dialog, you give a design variable a name and specify its properties.

The dialog has varying options depending on the type of design you are building and the type of variable you are adding.

Add Design Variable Dialog: Factorial or Plackett-Burman Design

Dialog: Add Design Variable (for a factorial design)



First, you give the design variable a name in the Name field. Each variable is given an ID letter (A, B, …), which you cannot change, as well as the name which you define.

Next, you choose whether the variable can vary continuously within a "Low to High" range (Continuous variable) or takes only a predefined number of values (Category variable) by selecting the appropriate radio button in the section Data Type.

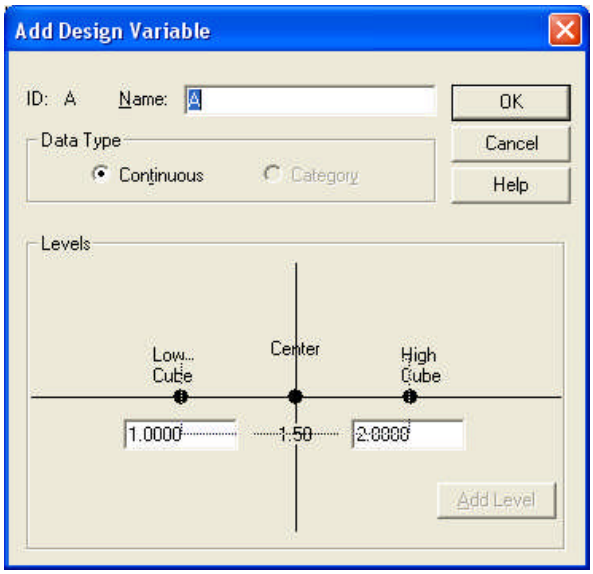
Finally, you specify the value of the design variable at the different levels of the design in the field Level. If a continuous variable is chosen, the values are entered in boxes in a graphical view of the design. For full factorial designs, you are allowed to define more than two levels, by clicking Add level. If you have chosen data type "category", the bottom of the dialog shows a list which by default contains two levels. Choose a level in the list, and fill in its name in the box below the list. You may add more levels to the design variable by clicking Add, or change the position of a level in the list by using Move up or Move down.

Note: Only two levels are allowed in fractional factorial and Plackett-Burman designs. Up to 20 levels are allowed in full factorial designs.

Add Design Variable Dialog: Box-Behnken Design

The dialog has about the same shape as for a factorial design (see Add Design Variable Dialog: Factorial or Plackett-Burman Design) but in addition, the Center level is displayed.

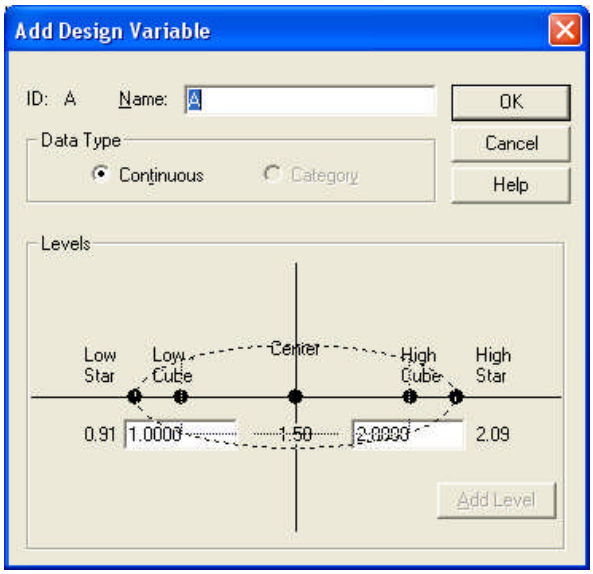
Dialog: Add Design Variable (for a Box-Behnken design)



Add Design Variable Dialog: Central Composite Design

The dialog has about the same shape as for a factorial design (see Add Design Variable Dialog: Factorial or Plackett-Burman Design) but in addition, the Low Star, Center and High star levels are displayed.

Dialog: Add Design Variable (for a Central Composite design)

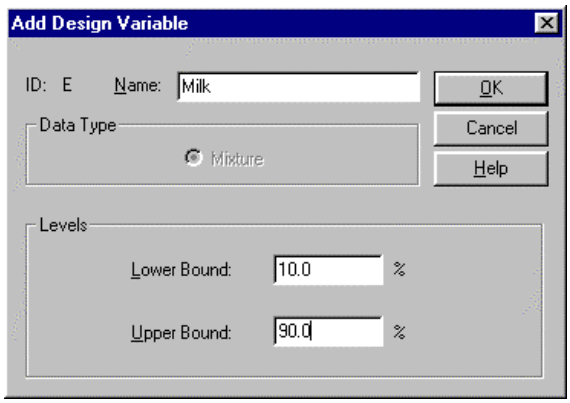


Star points are used in Central Composite designs only. The star point values are calculated automatically, depending on the number of design variables. After you have defined all your design variables, you may change the star distance to center in the **Define Design Variables** dialog. This is useful when a star point is placed in an invalid area, e.g. negative concentration. Using another distance than the default distance, however, changes the statistical properties of the design. Be careful not to change that distance if you do not have to.

Add Design Variable Dialog: Mixture Variable

Give the new mixture variable a name and specify its lower and upper bounds. Press OK.

Dialog: Add Design Variable (for Mixture variables)



Add Design Variable: Process Variable

The shape of this dialog is similar to the case of a factorial design (see Add Design Variable Dialog: Factorial or Plackett-Burman Design).

Design Wizard - Define Non-design Variables

Here, you specify responses, non-controlled variables, or variables with constant value. The values of these variables are simply recorded during the experiments.

Click New to create a new variable.

Note: Once the design is built, you will still have the opportunity to create new non-design variables in the Editor (**Edit - Insert - Variable** or **Edit - Append - Variables**).

Add Non-design Variable

When you click respectively New or Properties in the **Define Non-design Variables** dialog, you enter a dialog called **Add Non-design Variable** or **Variable Properties** respectively. Here, the non-design variables are numbered automatically, and you simply choose a name for the variable.

Define Non-design Variables - Next Dialog

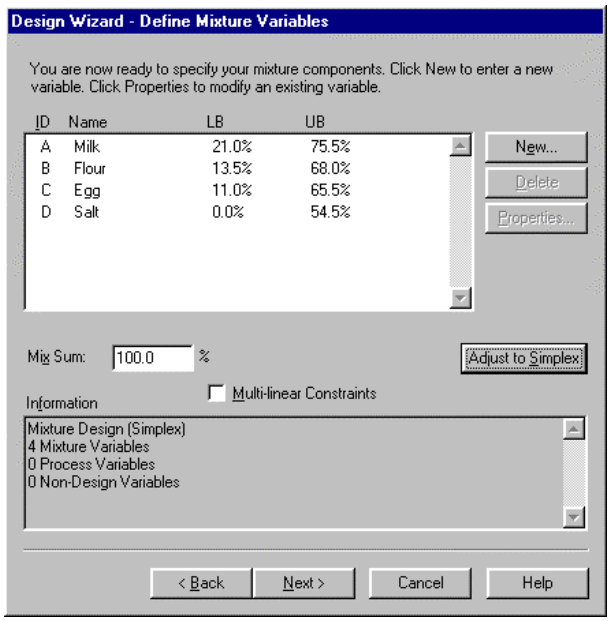
Once you have added all necessary non-design variables by clicking New or changed their definitions by clicking Properties, you may proceed by clicking Next. You will then access the next dialog, which varies depending on the type of design you are building:

- Full Factorial, Plackett-Burman, Central Composite or Box-Behnken: **Design Details**
- Fractional Factorial: **Design Type**
- D-optimal Non-mixture, Mixture design: **Define Model**

Design Wizard - Define Mixture Variables

In this dialog, you define the mixture variables that you want to investigate in your design.

Design Wizard: Define Mixture Variables



A Mixture variable is a variable whose quantity is linked to other variables in a mixture. Increasing the quantity of A in a mixture of four ingredients will imply decreasing the quantity of B, C and/or D in order to keep the total mixture amount constant.

Note: You must define at least three mixture variables in this dialog. If you are mixing only two ingredients together, build a classical non-mixture design (factorial, etc.) and define the percentage of one of the ingredients in the mixture as a design variable.

The dialog allows you to add a new or to delete or change an already defined variable by clicking one of the buttons New, Delete or Properties. Clicking New or Properties leads you to the **Add Design Variable** (or **Variable Properties**) dialog where you can specify the name and properties of the mixture variable.

In the MixSum field, select the total amount of your mixed ingredients (between 0% and 100%, or between 0 and 1 depending on the mixture component unit). Set this value lower than 100% (res. 1) if a constant part of the mixture is not modeled.

Note: You can choose to express the MixSum and the Lower and Upper Bounds either in percentages or fractions. This option is called Mixture Component Unit; it is found in the menu **File - System Setup - Editor**. This cannot be done while you are in the design wizard; exit to do it, then start the design wizard again with **File - New Design**.

Press the Adjust to Simplex button if you want to work with a simplex-shaped experimental region (classical Mixture design). The settings for lower and upper bounds will be adjusted to create a simplex region. Otherwise, if your experimental region is not a simplex, a D-Optimal design will be generated.

Note: Adjust your design to a simplex region if you want to include category variables.

Check the Multi-Linear Constraints checkbox if you want to include multi-linear constraints on your variables.

Define Mixture Variables - Next Dialog

Once you have added all necessary mixture variables by clicking New or changed their definitions by clicking Properties, you may proceed by clicking Next. Depending on your choices, the next dialog will be the following:

- If you checked the Multi-Linear Constraints checkbox: **Enter Multi-Linear Constraints**

- If not: **Define Process Variables**

Design Wizard - Define Process Variables

In this dialog you can define your non-mixture design variables.

The top field displays information about all defined design variables, while the Information field displays information about the currently selected variables and design.

The dialog allows you to add a new or to delete or change an already defined variable by clicking one of the buttons New, Delete or Properties. Clicking New or Properties leads you to the **Add Design Variable** (or **Variable Properties**) dialog where you can specify the name and properties of the process variable.

If two or more of your variables are linked by a linear relationship, check the Multi-Linear constraints box and click Next.

Define Process Variables - Next Dialog

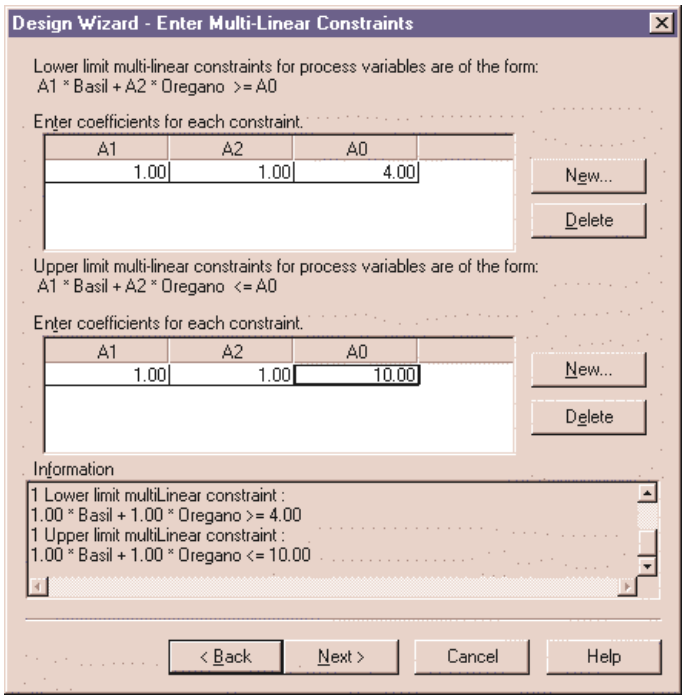
Once you have added all necessary process variables by clicking New or changed their definitions by clicking Properties, you may proceed by clicking Next. Depending on your choices, the next dialog will be the following:

- If you checked the Multi-Linear Constraints checkbox: **Enter Multi-Linear Constraints**
- If not: **Define Non-design Variables**

Design Wizard - Enter Multi-Linear Constraints

In this dialog, you can define up to 20 constraints between your process or mixture variables. If a constraint falls out of the experimental region, an information dialog opens, warning you that you have either to change this constraint or remove it from the design specifications.

Dialog: Design Wizard - Enter Multi-Linear Constraints



The upper part of the dialog is used to define Lower limit constraints, i.e. constraints of the form:
A1* DesignVariable1 + A2 * DesignVariable2 + … ≥ A0
The actual names of your design variables are displayed in text format.

The lower part of the dialog is used to define Upper limit constraints, i.e. constraints of the form:
A1* DesignVariable1 + A2 * DesignVariable2 + … ≤ A0
The actual names of your design variables are displayed in text format.

Click on the New… buttons to initiate the definition of new constraints. Then, type in the coefficients A1, A2, A3,… and the constant A0.

Use the Delete button to delete unwanted constraints. At the bottom of the Information field, you may view the defined constraints. Click for example Next and Back again to update the Information field with the latest defined constraints.

Notes:

- Multi-linear constraints automatically lead to a D-Optimal design (Mixture and Non-Mixture).

- One multi-linear constraint cannot involve both mixture and process variables.

- No multi-linear constraints can be defined in a design including category variables.

- Multi-linear constraints are not available in non-designed data tables

Enter Multi-Linear Constraints - Next Dialog

Once you have added all desired constraints, you may proceed by clicking Next. You will then access the next dialog **Define Non-design Variables**.

Design Wizard - Define Model

This dialog allows you to include interaction and square effects in a D-Optimal design or in a simplex Mixture design. Four predefined sets of effects are shown:

- Mixture Interactions and Squares
- Process Interactions
- Process Squares
- Mixture and Process Interactions

In the case of a D-Optimal Non-mixture design, the checkboxes related to mixture variables are disabled.

Besides, interactions and/or squares may be disabled depending on the number of defined process variables. For more than 6 variables, no squares can be included; for more than 9 variables, no I&S can be included in the model.

By clicking the Modify button, you enter the **Interaction and Square Effects Selection** dialog (see detailed description below).

Here are three basic rules regarding Mixture Designs:

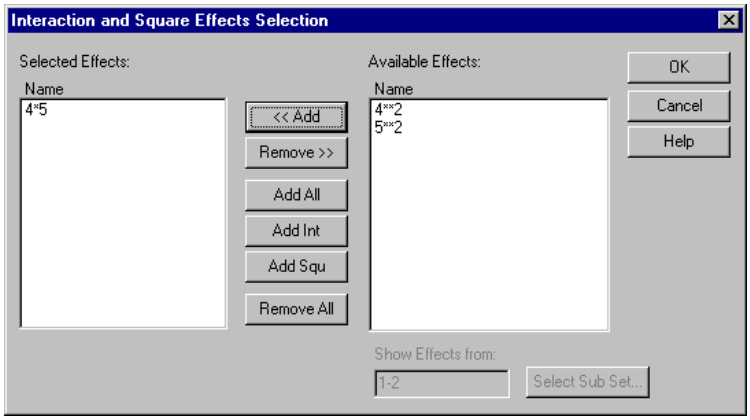
1. In a Mixture Design with additional process variables, ***process variable squares*** may be included only if your ***continuous process variables*** have ***more than two*** levels.
2. An ***interaction*** between a ***process*** variable and a ***mixture*** variable can only be added together with the set of ***all interactions*** between the same process variable and every mixture variables.
3. Interaction and square effects ***among mixture variables*** can only be added as a ***complete set***, that is, all the I&S effects together can be added/removed from the variable set, no individual selection is allowed.

Interaction and Square Effects Selection

In this dialog, you can select the interactions and squares that you wish to include in the model without taking a whole predefined set.

The dialog box contains two lists; Selected Effects to the left and Available Effects to the right. The latter lists all available effects with their full names. Select the ones you wish to include and press the Add button to include them in the leftmost list under short names. You can also Add All, Add Int (i.e. Interaction Effects) and Add Squ (i.e. Square Effects). Use the Remove or Remove All buttons to remove effects from the leftmost list. If your Variable Set contains more than 64 variables, you must push the Select sub-set button to define a set with max. 64 variables before you can select effects.

Dialog: Interaction and Square Effects Selection



Define Model - Next Dialog

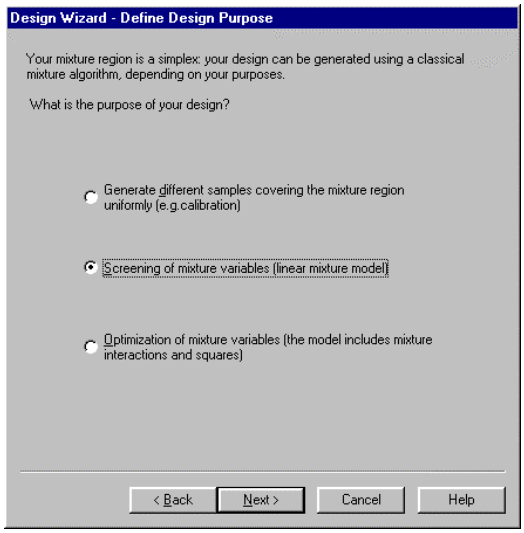
Once you have added all desired effects to your model, you may proceed by clicking Next. Depending on your type of design, the next dialog will be as follows:

- D-optimal Non-mixture or Mixture: **Design Details**
- Mixture with a simplex region (with or without Process variables): **Define Design Purpose**

Design Wizard - Define Design Purpose

In this dialog, which is specific to a Mixture Design with a simplex experimental region, specify the purpose of your design by selecting the proper radio button: calibration, screening or optimization.

Design Wizard: Define Design Purpose


Design Wizard - Define Design Purpose
Your mixture region is a simplex: your design can be generated using a classical mixture algorithm, depending on your purposes.
What is the purpose of your design?
Generate different samples covering the mixture region uniformly (e.g.calibration)
Screening of mixture variables (linear mixture model)
Optimization of mixture variables (the model includes mixture interactions and squares)
< Back
Next >
Cancel
Help

Note: An ***optimization*** design implies that square terms of mixture variables are included in the model. This radio button will also be disabled if too many variables are included in the model: in this case, it is necessary for you to go through a screening stage to identify the influential variables before you start an optimization.

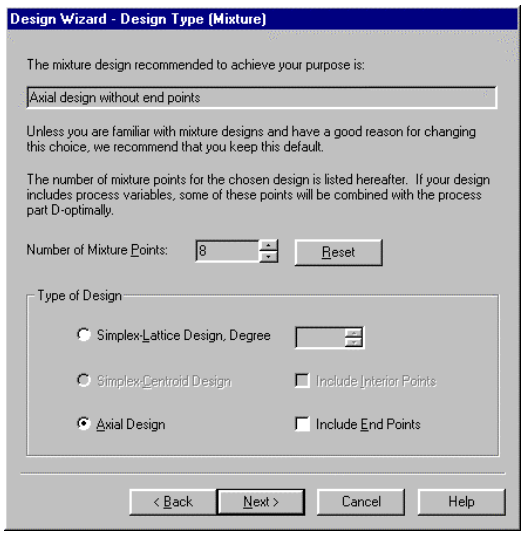
Define Design Purpose - Next Dialog

Once you have chosen the purpose of your design, you may proceed by clicking Next. You will then access the next dialog **Design Type (Mixture)**.

Design Wizard - Design Type (Mixture)

This dialog is specific to mixture designs with a simplex experimental region. In this dialog, you can choose the kind of Mixture Design that you want to use (Simplex-Lattice, Centroid or Axial), as well as the settings for these designs (Lattice degree, inclusion or not of Interior or End points). A recommended choice is displayed, and unless you have a particular reason not to follow the advice, you should follow it.

Design Wizard: Design Type (Mixture)


Design Wizard - Design Type (Mixture)
The mixture design recommended to achieve your purpose is:
Axial design without end points
Unless you are familiar with mixture designs and have a good reason for changing this choice, we recommend that you keep this default.
The number of mixture points for the chosen design is listed hereafter. If your design includes process variables, some of these points will be combined with the process part D-optimally.
Number of Mixture Points:
8
Reset
Type of Design
Simplex-Lattice Design, Degree
Simplex-Centroid Design
Include Interior Points
Axial Design
Include End Points
< Back
Next >
Cancel
Help

The Reset button brings back the system defaults for all fields.

Note: In a Simplex-Lattice Design of degree >2, all interaction and square effects can be included in the model. For degrees 1 and 2, only interactions between process variables and mixture variables are allowed.

Design Type (Mixture) - Next Dialog

After choosing a mixture design type in the **Design Type (Mixture)** dialog, you enter the next dialog: **Design Details**.

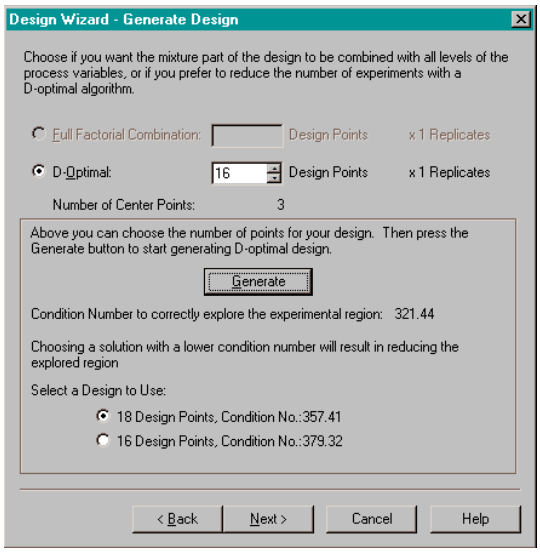
Design Wizard - Generate Design

This applies to D-optimal designs only.

This dialog gives you access to D-Optimal design generation. Note that it contains a radio button (Full Factorial Combination) which is related to the case of a Mixture Design; this button is disabled in the case of a Non-mixture design.

Generate Design - D-optimal Non-mixture

Design Wizard: Generate Design (D-Optimal non-mixture situation)


Design Wizard - Generate Design
Choose if you want the mixture part of the design to be combined with all levels of the process variables, or if you prefer to reduce the number of experiments with a D-optimal algorithm.
Full Factorial Combination:
Design Points
x 1 Replicates
D-Optimal:
16
Design Points
x 1 Replicates
Number of Center Points:
3
Above you can choose the number of points for your design. Then press the Generate button to start generating D-optimal design.
Generate
Condition Number to correctly explore the experimental region: 321.44
Choosing a solution with a lower condition number will result in reducing the explored region
Select a Design to Use:
18 Design Points, Condition No.:357.41
16 Design Points, Condition No.:379.32
< Back
Next >
Cancel
Help

In the upper field, choose the number of design points that you want by operating the spin button. The default number of design points is:

- Screening designs (no square terms): P+4
- Optimization designs (square terms): P+6

where P is the number of design variables, interaction terms and square terms in the model.

This default number allows a correct estimation of the experimental error. However, if you really need to perform fewer experiments, the system will let you decrease this number down to: P+1 for a screening design, and P+4 for an optimization design. On the contrary, if you can make do with more experiments, increase this default number to gain accuracy.

Note: When choosing the number of design points, keep in mind that this number does not include center and reference samples, and must be multiplied by the number of replicates to obtain the real number of experiments you will have to produce.

After selecting the number of design points, press Generate to let the system start the D-optimal algorithm. The system generates four designs with a number of design samples equal to or close to your request (from -1 to +2 experiments).

The best two designs (lowest Condition No.) are displayed in the lower field. Choose which one to use according to this rule: the closer the Condition no. is to 1, the better. The condition number necessary to correctly explore your experimental region is automatically computed and displayed in the dialog text. When reaching substantially higher condition numbers, we recommend not using the design: it will not cover the experimental region correctly, but will describe some variables and let aside other ones.

Note: If the two designs displayed do not suit you, press Generate again. The Unscrambler will generate four new designs, and will compare them to the former ones before displaying the two best solutions. Press Generate several times to give The Unscrambler a better chance to generate a good design for your purposes.

Generate Design - Mixture

When building a Mixture design, this dialog is accessed in the two following cases:

- The experimental region is not a simplex;

- The experimental region is a simplex and the design includes Process variables.

These two cases are treated differently; they are exposed hereafter.

The experimental region is not a simplex

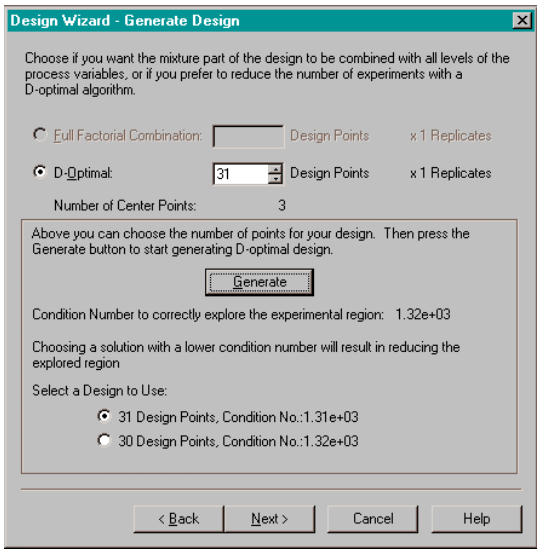
If the experimental region of your Mixture design is not a simplex (for instance, if you defined Multi-Linear constraints), a D-Optimal design will be generated. The process is the same as in the case of a D-Optimal Non-mixture design (see Generate Design - D-optimal Non-mixture).

The experimental region is a simplex and the design includes Process variables

In this situation, The Unscrambler offers you the choice between:

- combining all points of the simplex mixture design with all combinations of levels of the process variables: tick the radio button Full Factorial Combination
- reducing the number of experiments by using the D-optimal algorithm: tick the radio button D-Optimal.

Design Wizard: Generate Design (Mixture situation)


Design Wizard - Generate Design
Choose if you want the mixture part of the design to be combined with all levels of the process variables, or if you prefer to reduce the number of experiments with a D-optimal algorithm.
Full Factorial Combination:
Design Points
x 1 Replicates
D-Optimal:
31
Design Points
x 1 Replicates
Number of Center Points:
3
Above you can choose the number of points for your design. Then press the Generate button to start generating D-optimal design.
Generate
Condition Number to correctly explore the experimental region: 1.32e+03
Choosing a solution with a lower condition number will result in reducing the explored region
Select a Design to Use:
31 Design Points, Condition No.:1.31e+03
30 Design Points, Condition No.:1.32e+03
< Back
Next >
Cancel
Help

Try the two radio buttons and compare the properties of the two designs in order to make up your mind: the information displayed gives you the required number of experiments as well as the condition number for the selected design. This information is computed from all your former settings, in particular it takes into account the Interaction and Square terms that you included in the Define Model dialog.

Refer to Generate Design - D-optimal Non-mixture (p.114) for complementary information on the generation of a D-Optimal design in this dialog.

Generate Design - Next Dialog

Once you have selected the suitable options, and if you chose a D-optimal solution, only after you have pressed Generate and are satisfied with the result, you may press Next. The next dialog depends on the specifications of your design:

- If some of the variables are constrained: **Last Checks**

- Otherwise: **Randomization Details (General)**

Design Wizard - Design Type

This applies to Fractional Factorial designs only.

When you have specified all non-design variables, you proceed to the dialog **Design Type**, where you specify either the **Resolution** you wish to achieve or the **Number of Experiments** you can run. If you choose to specify the resolution, The Unscrambler will automatically create a design with as few experimental runs as possible. If you specify the number of experimental runs, it will choose the design with the highest possible resolution.

The first field of the dialog, Number of experiments to run, displays how many experimental runs the chosen design will require, excluding replicates and possible center and reference samples, which you may define later on.

The field Resolution displays the resolution of the selected design. Change the resolution by clicking the appropriate radio button.

In the field Confounding Pattern, the confoundings are shown for the current design, as a list. Effects which cannot be studied independently from each other are displayed on the same line of the list. For example, A = BC = DE means that the main effect or A is confounded with the interaction between B and C, and the interaction between D and E.

Effects up to three-variable interactions are displayed on the list. However, you should not worry too much about three-variable interactions, since they are usually negligible. What matters most is whenever main effects and two-variable interactions are confounded with each other.

The generators of the design are shown in the Information field.

Details on Resolution and Confoundings

The confoundings for the various resolutions available in the dialog **Design Type** are shown below.

Resolutions and confoundings for various types of designs

Resolution	Confoundings
Resolution III	Main effects are not confounded with each other. Main effects are confounded with two-variable interactions.
Resolution IV	Main effects are not confounded with each other. Main effects are not confounded with two-variable interactions. Two-variable interactions are confounded with each other
Resolution V	Main effects are not confounded with each other. Main effects are not confounded with two-variable interactions. Two-variable interactions are not confounded with each other. Two-variable interactions are confounded with three-variable interactions. Three-variable interactions are confounded with each other.

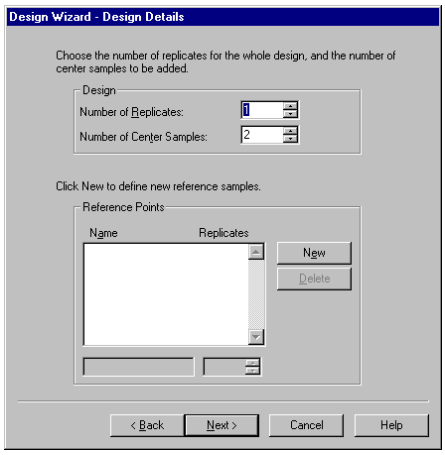
Design Type - Next Dialog

Once you are satisfied with your choice, press Next to enter dialog **Design Details**.

Design Wizard - Design Details

This dialog allows you to specify details related to replicates, Center samples and Reference samples.

Dialog: Design Details



In the field Design you choose the number of replicates and center samples.

The Number of Replicates indicates the number of times the main experiments are run. Increasing the number of replicates gives more precise estimates of the effects due to better coverage of the experimental error. Use at least two replicates if you know that your experimental results are likely to vary from time to time. The Unscrambler only supports balanced designs, so the number of replicates must be the same for all design points.

Note: Replicates are not the same as ***repeated measurements***. Replicates mean that a new experiment is run using the same settings for the design variables as in a previous one, while repeated measurements means measuring the response values for the same experiment several times .

The Center Samples are samples located in the center of the design. This is only possible if all the variables are 2-level and continuous. Center samples are used for curvature checking and for error variance estimation. Use at least 2 (preferably 3 or more) center samples. The location is defined by the levels of the factorial design variables. The center samples correspond to the average (mean) of the different variables in the design.

In the field Reference Points you define samples which are incorporated for comparison. A typical reference sample is a target sample, a competitor's sample or a sample produced after to a given recipe. The values of the design variables are not entered and are set as missing.

Design Details - Next Dialog

Once you are satisfied with your choice, press Next to enter dialog **Randomization Details (General)**.

Design Wizard - Randomization Details (General)

Sometimes it is useful to perform some experiments in sequence. For example, the temperature may be very difficult to change, so you want to make all experiments with the same temperature at the same occasion. In the dialog **Randomization Details**, which you enter when you click Next in the **Design Details** dialog, you can specify blocks of similar samples to be kept together during randomization.

Your first option is to Keep reference samples together. Alternatively, you can select certain variables which are not to be randomized by selecting the appropriate variables in the section Available Variables and copying them to the Do Not Randomize section by clicking <<< or >>>.

Randomization Details - Next Dialog

Once you have made your selection and clicked Next, you access the last dialog of the Design Wizard: **Last Checks**.

Design Wizard - Last Checks

This is the last dialog, which gives you a summary of your design, now that it has been completely specified. Click Preview to see the randomized list of experiments. If you are not satisfied with the randomization, you can use Re-randomize. If the design is as you want is you may print a lab report by clicking Lab Report … .

Click Finish to end the design specification, or Back to review and alter your previous choices.

Clicking Finish makes you exit the design Wizard and displays the designed data table in the Editor. The design can then only be changed by way of **File - New Design - Modify existing design** (after giving it a name with **File - Save**).

The Edit Menu

Edit - Cut

or **Ctrl+X**

This option removes the selected range, either data in the Editor or a plot in the Viewer, and places it on the clipboard. Anything that you place on the clipboard remains there until you replace it with a new item.

You can restore your selection from the clipboard using the **Paste** command.

Edit - Copy

or **Ctrl+C**

With this option you copy the selected range to the clipboard, overwriting its previous contents. The selected range is with other words not removed from its original place. Use the **Paste** command to copy your selection to a new location.

Edit - Clear

This option is only enabled from a Viewer and clears it of all its contents, thus allowing you to make a new plot in the same Viewer.

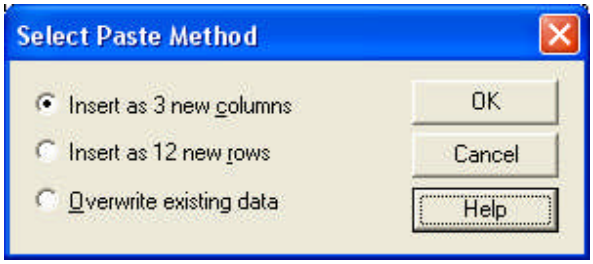
Edit - Paste

or **Ctrl+V**

Lets you insert a copy of the clipboard contents at the insertion point. The command is not available if the clipboard is empty or the selected range cannot be replaced.

When pasting data from another Windows application, the **Select Paste Method** dialog pops up.

Dialog: Select Paste Method

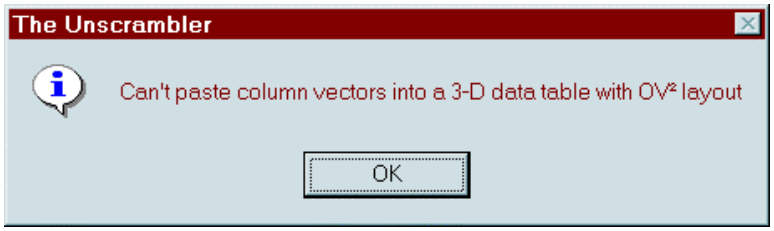


Make your choice and click OK.

Edit - Paste (3-D)

Pasting selections into a 3-D data table is restricted to the "unique" dimension in the table (rows in an OV^2 table, columns in an O^2V table). Attempts to paste column-oriented selections into an OV^2 table or row-oriented selections into an O^2V table will generate an error message.

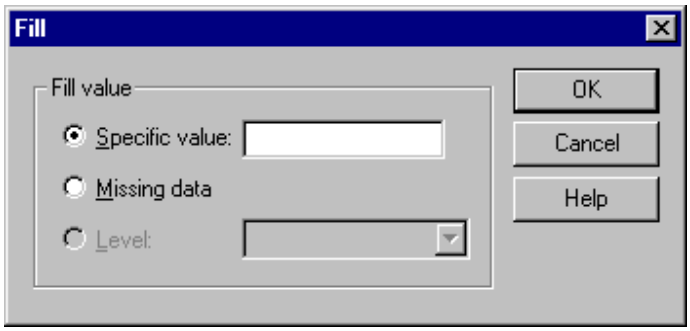
Error message upon illegal Paste



Edit - Fill

Here, you can fill the ***selected range*** with a value. You enter the dialog **Fill** where you can choose between Specific value, Missing data, or Level.

Dialog: Fill



The Level option is available only if the selected range spans non-designed category variables.

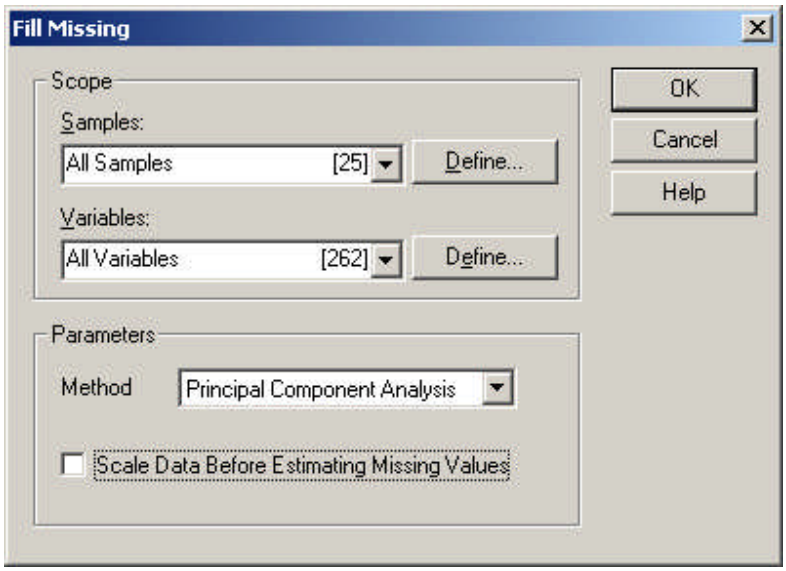
If the value you declare is invalid for some cells, these will not be filled.

Fill is not possible if the selected range contains locked cells, for example in a designed data table.

Edit - Fill Missing

Here, you can fill the ***missing values*** in your data table with estimated values that take into account the data structure.

Dialog: Fill Missing



In the **Fill Missing** dialog you can select the Scope (samples and variables) of the replacement. If necessary, click Define to access the **Set Editor**, which allows you to define new sets of samples or variables.

In the Parameters frame, choose the estimation Method:

- Principal Component Analysis will perform a reconstruction of the missing data based on a PCA model with an optimal number of components of the data selected in the scope field. This fill missing procedure is the default selection and the recommended method of choice for spectroscopic data.
- Row Column Mean Analysis will only make use of the same column and row as each cell with missing data. Use this method if the columns or rows in your data come from very different sources that do not carry information about other rows or columns. This can be the case for process data.

You may optionally Scale Data Before Estimating Missing Values by ticking the box at the bottom. This is recommended if the variables included in the replacement scope are measured in different units or have different scales.

Fill Missing - Difficult Situations

Filling missing values in a satisfactory way requires that the non-missing values in the table carry enough information for a reliable estimation.

The table hereafter lists the most frequent situations and their outcomes.

Table: Various situations and corresponding outcome of Edit - Fill Missing

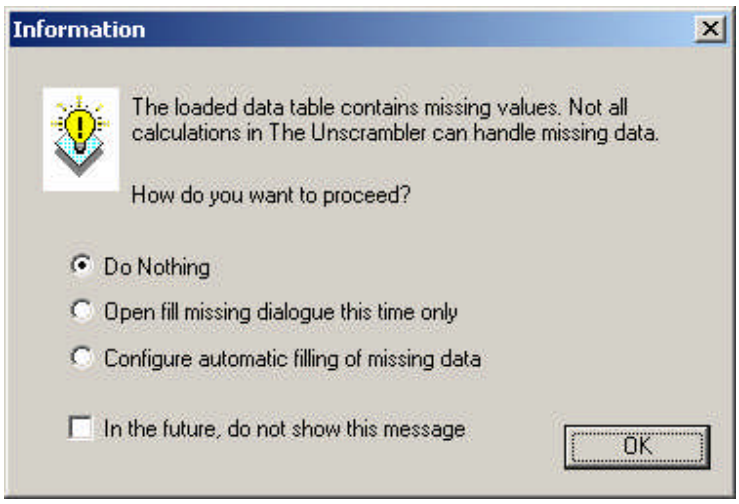
Situation	Problem	Outcome
No missing data	No cells to fill	Warning is displayed. No filling performed.
Some missing values, spread over several samples and variables	No problem	Filling is performed.
All values are missing in a row	No information available on that sample	Warning is displayed. Empty row is kept out of calculations.
More than 50% missing data in the table	Risk of unreliable estimation	Warning is displayed.

		Filling is performed.
All values are missing in the table	No information available at all	Warning is displayed. No filling performed.

Fill Missing - Information Dialog

Whenever you open a data table containing some missing values in the Editor, an **Information** dialog appears as shown below.

Dialog: Information (upon opening a data table with some missing values)


Information
The loaded data table contains missing values. Not all calculations in The Unscrambler can handle missing data.
How do you want to proceed?
Do Nothing
Open fill missing dialogue this time only
Configure automatic filling of missing data
In the future, do not show this message
OK

Choose between the three courses of action:

- Do Nothing: upon clicking OK, the data table is displayed in the Editor and nothing more is done.
- Open fill missing dialogue this time only: upon clicking OK, the **Fill Missing** dialog appears and helps you replace the missing values with estimated values.
- Configure automatic filling of missing data: upon clicking OK, the Missing Data sheet of **System Setup** dialog appears and helps you configure automatic replacement of missing values with estimated values in all data tables.

If you do not want the Information dialog to be displayed in the future, tick the box at the bottom of the dialog.

Note 1: If you choose to Configure automatic filling of missing data, the Information dialog will not be displayed in the future.

Note 2: If the Information dialog does not appear when you open a data table containing missing values, you may use **File - System Setup** and configure automatic filling of missing values. If you later on turn off that setting, the Information dialog will again appear whenever relevant.

Edit - Insert

Through this option, you gain access to 4 sub-options:

1. Insert Sample;

Insert Variable;

Options 1 and 2 are described in a common section:

2. Edit - Insert - Sample or Variable.
3. Insert Category Variable;
4. Insert Mixture Variables.

Edit - Insert - Sample

See

Edit - Insert - Sample or Variable (right below).

Edit - Insert - Variable

See

Edit - Insert - Sample or Variable (right below).

Edit - Insert - Sample or Variable

You can insert a variable or a sample in a given Editor. A new column is inserted to the left of the column containing the currently active cell. New rows are inserted above the active cell.

It is not possible to insert variables or samples between variables or samples in locked cells, e.g. in a designed data table.

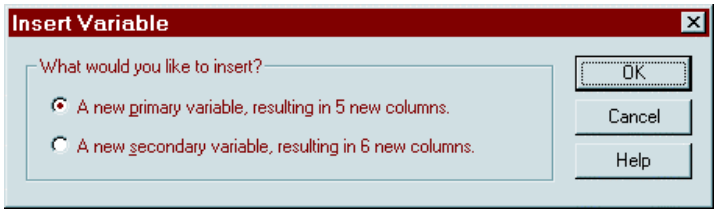
Inserted variables are always continuous. An inserted sample is assigned the same type as the sample above it. The cells are filled with 'm', indicating missing data, until you edit them.

Previously defined Sets are adjusted to accommodate the inserted range.

Insert Sample or Variable (3-D)

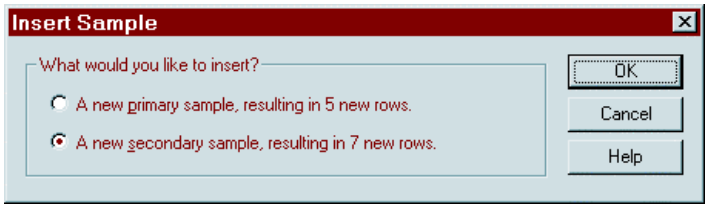
If your table has an OV^2 layout, you may insert either Primary or Secondary variables, as shown below. Samples can be inserted as in 2-D data.

Dialog: Insert Variable (OV^2)


Insert Variable
What would you like to insert?
A new primary variable, resulting in 5 new columns.
A new secondary variable, resulting in 6 new columns.
OK
Cancel
Help

If your table has an O^2V layout, you may insert either Primary or Secondary samples, as shown below. Variables or Category variables can be inserted as in 2-D data.

Dialog: Insert Sample (O^2V)


Insert Sample
What would you like to insert?
A new primary sample, resulting in 5 new rows.
A new secondary sample, resulting in 7 new rows.
OK
Cancel
Help

Edit - Insert - Category Variable

Here, you may insert a category variable, which is useful during interpretation of plots and to create groups on which to calculate statistics.

Note: You cannot insert a Category variable into a 3-D table with layout OV^2.

This option starts the Category Variable Wizard, which consists of the following dialogs:

Category Variable Wizard - Enter Variable Name and Choose Method

In the field Category variable name, you enter the name you want to give the variable in the data table. The name will be written in blue in the Editor to indicate that it is a category variable.

Then you can choose between specifying the levels of the variable manually or basing the levels on a collection of sample sets. The levels are the discrete values that are valid for that variable.

Select the appropriate radio button and press Next to go to the next dialog, which will depend on your choice of method:

- If you selected “manually”, the next dialog is **Specify Levels**
- If you selected “collection of sample sets”, the next dialog is **Select Sets**

Category Variable Wizard - Specify Levels

This dialog lets you specify your levels manually.

To ***create a new level***:

1. Type in the name of the new level in the empty field to the left of the Add button;
2. Press Add to validate the new level.

To ***change a level name***: double-click on that level on the list and type in a new name, then click anywhere inside the dialog box to validate the change.

You may also ***remove*** a level by selecting it from the list and clicking Remove, or ***change the order*** of the levels with the Move Up and Move Down buttons.

Note: The order of the levels in the list is important; it determines in which order the levels will be stored in The Unscrambler, which color will be associated to each level if you use Sample Grouping on a plot, etc.

When you are satisfied, click Finish to exit the Category Variable Wizard and go back to the Editor. You may then select the proper level of your new category variable for each sample.

Category Variable Wizard - Select Sets

You enter this dialog if you want to base the levels of the category variable on a collection of sample sets. Simply select the sets you want in the field Available Sets.

The selected sets must not be overlapping. The category variable will have as many levels as selected sets. The levels will take their names fom the selected sets, and each sample will automatically get the correct level. Samples which are not part of any selected sample set will have a missing value for the category variable.

When you are satisfied, click Finish to exit the Category Variable Wizard and go back to the Editor.

Edit - Insert - Mixture Variables

This function adds mixture variables to a non-designed data table. It is not available to designed data tables. When choosing this option, you are asked for a number of variables to add. After the insertion, the total number of mixture variables in the table has to be three or more.

Note1: If you want to insert a mixture variable to a designed data table, duplicate your table as non-design by selecting the menu option File - Duplicate - As Non-Design. Then you will be able to insert mixture variables to your table.

Note2: You cannot insert Mixture variables into a 3-D table.

Edit - Append

Lets you extend your data table with new samples or variables. You have 4 choices:

1. Append Samples;
2. Append Variables;

   Options 1 and 2 are described in a common section: Edit - Append - Samples or Variables.
3. Append Category Variable;
4. Append Mixture Variables.

Edit - Append - Samples

See Edit - Append - Samples or Variables (right below).

Edit - Append - Variables

See Edit - Append - Samples or Variables (right below).

Edit - Append - Samples or Variables

You enter the dialog **Append Samples** or **Append Variables**, where you use the spin button to select the number of samples or variables to add and click OK.

The new samples are inserted below the current last sample.

The new variables are inserted to the right of the last variable, and are of continuous non-design type.

All the new data cells are filled with the value “missing”.

Append Samples or Variables (3-D)

If your table has an OV^2 layout, you may append either Primary or Secondary variables. Select the number of variables to append and their type, then click **OK**. Samples can be appended as in 2-D data.

If your table has an O^2V layout, you may append either Primary or Secondary samples. Select the number of samples to append and their type, then click **OK**. Variables or Category variables can be appended as in 2-D data.

Edit - Append - Category Variable

Here, you may append a category variable, which is useful during interpretation of plots and to create groups on which to calculate statistics.

Note: You cannot append a Category variable to a 3-D table with layout OV^2.

This option starts the Category Variable Wizard, which consists of the following dialogs:

- Category Variable Wizard - Enter Variable Name and Choose Method
- Category Variable Wizard - Specify Levels
- Category Variable Wizard - Select Sets

Edit - Append - Mixture Variables

This function adds mixture variables to a non-designed data table. It is not available to designed data tables. When choosing this option, you are asked for a number of variables to add. After the insertion, the total number of mixture variables in the table must be three or more.

Note: If you want to append a mixture variable to a designed data table, duplicate your table as non-design by selecting the menu option File - Duplicate - As Non-Design. Then you will be able to append mixture variables to your table.

Note: You cannot append Mixture variables to a 3-D table.

Edit - Delete

or <Del>

This option only applies when you have selected one or more variables or samples, and deletes the selected section(s).

Variables or samples with locked cells cannot be deleted. Any previously-defined sets are adjusted for the deleted range.

You will be warned before deletion occurs if you have specified this option in the **System Setup** dialog.

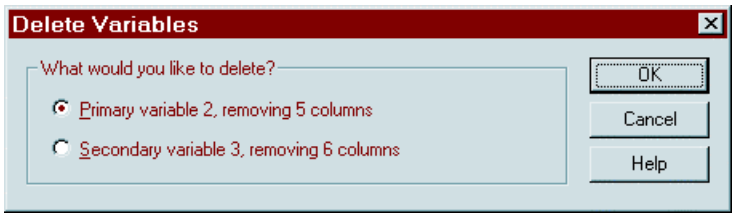
Edit - Delete (Mixture Variable)

This menu option can be used to delete mixture variables. It will fail for any variable selection that would leave only one or two mixture variables in the table after the deletion.

Edit - Delete (3-D)

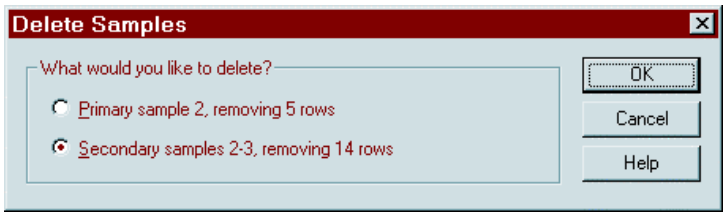
If your table has an OV^2 layout, you may delete either Primary or Secondary variables, as shown below. Samples can be deleted as in 2-D data.

Dialog: Delete Variables (OV^2)



If your table has an O^2V layout, you may delete either Primary or Secondary samples, as shown below. Variables and Category variables can be deleted as in 2-D data.

Dialog: Delete Samples (O^2V)



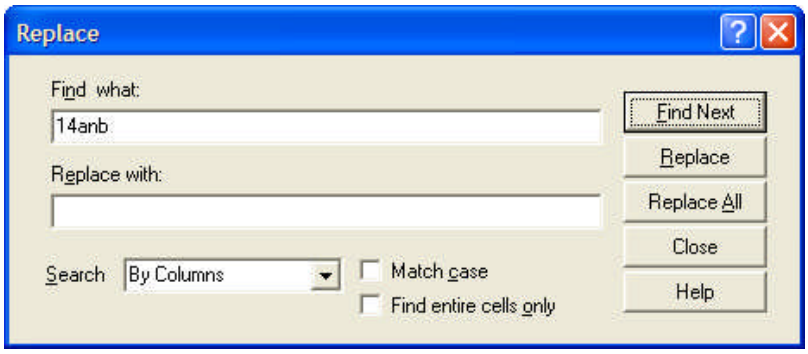
Edit - Find/Replace…

Ctrl+F

This command allows you to find cells containing a given value or sequence of characters, and replace the selected value with a new one.

Edit - Find/Replace… or **Ctrl+F** launches the **Replace** dialog, where you can specify the value to search for, launch the search, and optionally define a replacement value and perform the replacement.

Dialog: Replace



How to Find a value

In the Find what field, type in the value or sequence of characters to be searched for. By default, this field contains the value of the current cell. Any combination of digits and characters is allowed, e.g. “A51-02.b.DSF24%”.

To locate the chosen the value or sequence of characters in a cell, hit the Find Next button. If the search is successful, the cell is marked in the Editor with a black frame (or a white frame if the search is occurring in a selected area). If no match is found, a message is displayed.

You may change the direction of the search by toggling the Search field (either “By Columns” or “By Rows”).

In addition, two tick-boxes allow for a more specific search:

- Match case makes a difference between lower-case (e.g. “a”) and upper-case (e.g. “A”). This is relevant for Category variables only.
- Find entire cells only searches for cells which have the requested sequence of digits or characters as exact contents.

How to Replace a value with another

Once you have typed in a Find what value, you may proceed with a replacement.

In the Replace with field, type in the new value or sequence of characters. Any combination of digits and characters is allowed, e.g. “A51-02.b.DSF24%”. However, if the requested value is not compatible with the current type of cell (e.g. “A51” in a numeric cell), an error message will be displayed and no replacement will be made when you hit one of the Replace buttons.

If the Find what value has already been located with the Find Next button, hit the Replace button to replace the value in the current cell.

If you wish to make the replacement in all cells containing the Find what value, hit the Replace All button.

How to Undo Replace

Exit the **Replace** dialog and use command **Modify - Undo Replace**.

General features

The Close button closes the dialog.

The Help button launches the Help system on the relevant page.

Note: If some rows or columns of the data table are selected before using the **Edit - Find/Replace…** command, the search is performed ***only in the selected area***.

Note: only the ***cells*** of the data table are affected by this command. You cannot find or replace values located in the row or column headers (Sample names or Variable names).

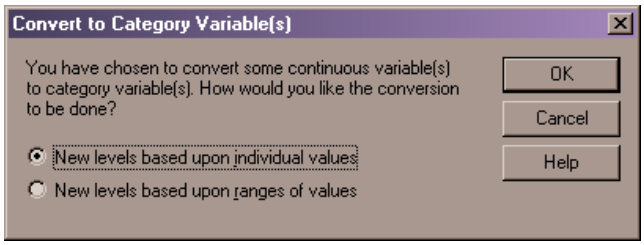
Edit - Correct Mixture Components

This function is specific to designed tables. It is available only when one or more mixture variables are selected. This function corrects the selected mixture variables so that the sum per row (i.e. per experiment) of all Mixture variables is equal to the MixSum value. The values in the non-selected mixture variables remain fixed during the operation.

Edit - Convert to Category Variable

In the Editor, highlight one or several columns containing continuous variables, and choose **Edit - Convert to Category Variable**. This launches the **Convert to Category Variable** dialog, where you can select a relevant conversion principle.

Dialog: Convert to Category Variable(s)


Convert to Category Variable(s)
You have chosen to convert some continuous variable(s) to category variable(s). How would you like the conversion to be done?
New levels based upon individual values
New levels based upon ranges of values
OK
Cancel
Help

Note: This option is disabled for 3-D data tables with an OV^2 layout.

Convert Individual Values into Levels

If you choose the first option, the values of the source variable will be sorted in increasing order, and each value will be assigned a level index accordingly.

Visually, the only obvious change in the Editor is the blue variable name, and the left justified cell values.

Warning!

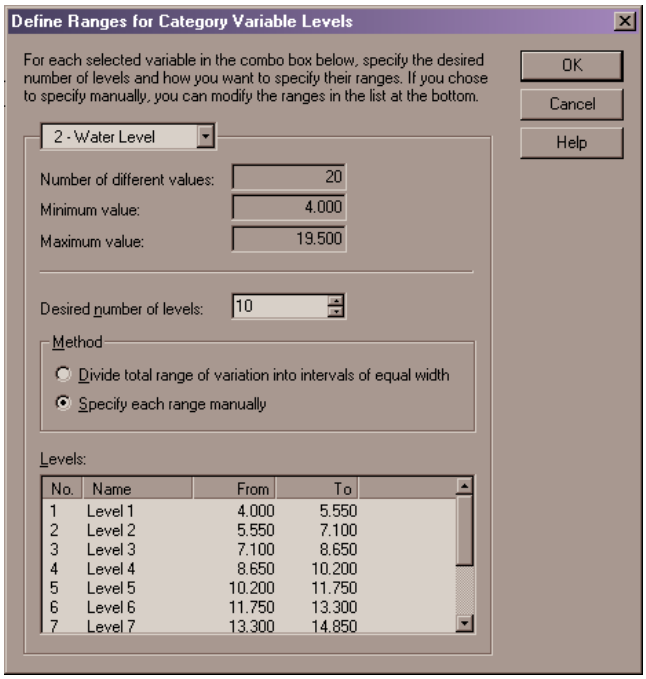
If the source variable has more than 20 different values, the remaining values after sorting and affecting level indices 0-19 will be replaced by “m” (missing).

Convert Ranges of Values into Levels

If you choose the second option, the values of the source variable will be sorted in increasing order and affected to a range of values between a lower and an upper limit. Each interval will then become a new level.

The **Define Ranges for Category Variable Levels** dialog allows you to specify those ranges for each of the variables to be converted.

Dialog: Define Ranges for Category Variable Levels


Define Ranges for Category Variable Levels
For each selected variable in the combo box below, specify the desired number of levels and how you want to specify their ranges. If you chose to specify manually, you can modify the ranges in the list at the bottom.
OK
Cancel
Help
2 - Water Level
Number of different values: 20
Minimum value: 4.000
Maximum value: 19.500
Desired number of levels: 10
Method
Divide total range of variation into intervals of equal width
Specify each range manually
Levels:
No. Name From To
1 Level 1 4.000 5.550
2 Level 2 5.550 7.100
3 Level 3 7.100 8.650
4 Level 4 8.650 10.200
5 Level 5 10.200 11.750
6 Level 6 11.750 13.300
7 Level 7 13.300 14.850

With the help of the combo-box, choose the variable for which you want to specify ranges.

The number of different values, together with the minimum and maximum values of that variable, are displayed below the combo-box. Check these values to help you make your choice in the options that follow.

Select the desired number of levels (between 1 and 20).

In the Method field, choose whether to divide the actual range of variation (from “Minimum value” to “Maximum value”) into intervals of equal width, or specify each range manually.

Intervals of equal width

The system automatically computes the lower and upper limit of each interval defining a new level. The levels are named “Level 1”, “Level 2”, etc.

Specify ranges manually

If you choose to specify each range manually, the list of levels, their names and ranges automatically generated can be changed by double-clicking on the item in the list. Tune your level names, lower and upper limits until you get the desired specification.

Once you have specified each variable, you may click OK. The selected variables will be converted accordingly.

Note: After conversion, you may use **Modify - Properties** in order to change the level names or add new levels. However, this will have no retroactive impact on level definition as related to the original continuous variable.

Warning!

The **Edit - Convert to Category Variable** command replaces the original continuous variable with the resulting Category variable. If you want to keep your original continuous variable in the table, use Copy and Paste *before* the conversion.

Edit - Convert to Mixture Variable

This function converts a set of non-designed continuous variables to mixture variables. The function is available only for non-designed data tables. A dialog opens, where you can select a set of variables to convert (e.g. the Selected Variables) and you can change the MixSum value before the variables are converted.

Note1: After converting your variables, you can use **Edit - Correct Mixture Components** so that all the mixture variables in your data table, the old ones as well as the newly converted ones, give a sum per experiment equal to MixSum.

Note2: The **Convert to Mixture Variables** option is disabled for all 3-D data tables.

Edit - Split Category Variable

Splits one category variable into several new (continuous) variables. There will be as many new variables as there were levels in the category variable. For example: a category variable with two levels, say A and B, gets an addition of two continuous variables labeled A and B. The samples are coded with +1 and 0 to indicate which level was used originally. The figure below illustrates the principle.

Splitting a category variable

Cat.var
A
A
B
B
C
C

⇒

A	B	C
+1	0	0
+1	0	0
0	+1	0
0	+1	0
0	0	+1
0	0	+1

This operation is irreversible and only available for non-designed category variables.

Edit - Go To

or **Ctrl+G**

Activates a specific cell in the data table. You enter the dialog **Goto**, where the field Row lets you choose which sample to go to by pressing the spin button, while the field Column works the same way when you want to go to a variable.

Edit - Go To (3-D)

Activates a specific cell in the data table. You enter the dialog **Goto**, where the field Row lets you choose which sample to go to by pressing the spin button, while the field Column works the same way when you want to go to a variable.

If your 3-D table has layout OV^2, the field Column is connected to two additional fields: Primary Var and Secondary Var. All three fields help you select the desired column in the most flexible way, as shown in the figure below.

Dialog: Go To for an OV^2 3-D table

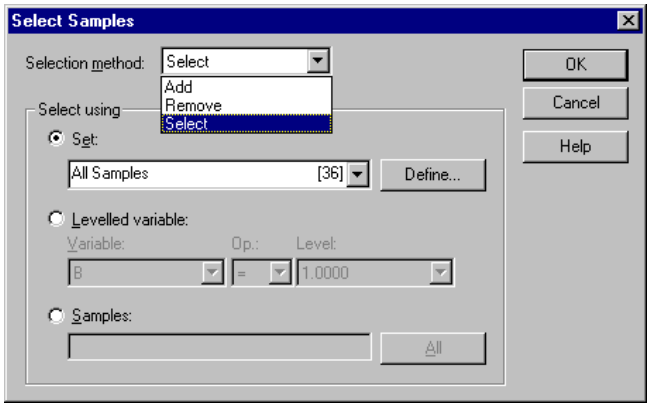
If your 3-D table has layout O^2V, the field Row is connected to two additional fields: Primary Sam and Secondary Sam. All three fields help you select the desired row in the most flexible way, as shown in the figure below.

Dialog: Go To for an O^2V 3-D table

Edit - Select Samples…

In the dialog **Select Samples**, you can choose which samples you want to work with as the sample set "Currently Selected Samples" in your analysis. You can extend or reduce the number of samples you work with at the moment.

Dialog: Select Samples



In the field Selection method, a drop-down menu gives you 3 options:

- Select: Selects the samples you specify.
- Add: Adds the samples you specify to the samples already selected.
- Remove: De-selects the samples you specify from the samples already selected.

In the next field, Select Using, you select 1 out of 3 available radio buttons; Set, Leveled variable, Samples

If you click Set, the new samples can be chosen from a predefined set. A set is defined by the **Edit Set** command in the **Modify** menu. The button Define next to the drop-down menu takes you to the dialog **Set Editor**, where you may review all available sample and variable sets and choose between samples and variables.

Clicking Leveled Variable allows you to base sample selections on the levels in some variables. The variable is defined in Variable and the level in Level. You determine whether the selected samples should be the samples with (=) or without (≠) the specified level(s).

Selecting Samples lets you specify the samples you want to select, add, or remove. Adjacent samples are indicated by a hyphen (e.g. 4-8 means 'samples 4, 5, 6, 7 and 8), while commas are used as delimiters in multiple selections, e.g. 1,4-8,10,15-25. If you want to select all samples, click the All button to the right of the field.

Edit - Select Variables…

In the dialog **Select Variables**, you may select the variables you want to work with as the variable set "Currently Selected Variables" in your analysis. You can increase or reduce the number of variables you are working with at the moment.

The field Selection method is identical to the one in the dialog **Select Samples**.

In the Select using field you select to use either an existing set, as in the **Select Samples** dialog, or variables which you specify.

Use the button All to specify all variables. Adjacent variables are specified with a hyphen, eg. 4-8; commas are used to separate multiple intervals, eg. 1,4-8,10,15-25.

Edit - Select All

You can use this command to select the entire matrix. The next operation you choose will be performed on all elements in the matrix.

Note: The Unscrambler always works with either rows or columns. This also applies when the whole matrix is selected. Look at the cursor shape or the rows/columns numbers to see whether you are in row or column mode. Sample names will also be selected if you are in sample mode, and vice versa.

Edit - Adjust Width

or **Ctrl+W**

Adjusts the width of selected columns to exactly fit all data values.

If you want this command to also take variable names into account when adjusting the column width, this must be specified in the **System Setup** dialog.

Edit - Add Plot…

or **Ctrl+A**

In the General Viewer, **Edit - Add Plot** allows you to add a second plot of the same type as the one(s) already displayed.

This command is also available through the shortcut CTRL-A.

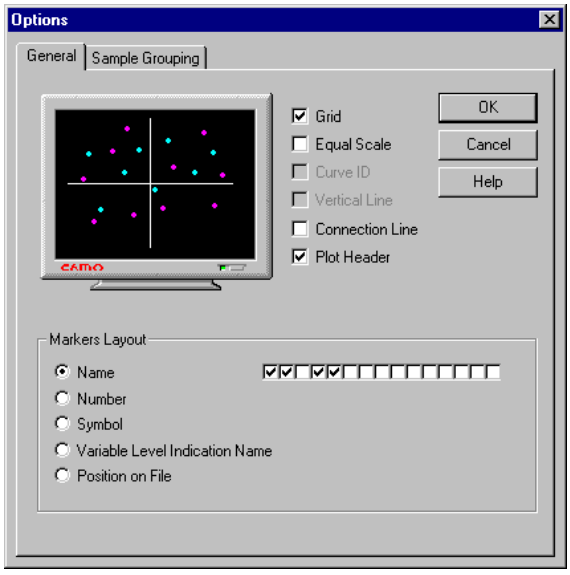
Note: This command can only be applied to plots of the following types: Line, 2D scatter and 3D scatter.

Edit - Options…

or **Ctrl+L**

You can use this command to change the appearance of the plot you are working on. The **Options** dialog always contains the sheet General; in addition, the sheet Sample Grouping is available in predefined plot mode when you display a sample oriented plot, e.g. a score plot.

Dialog: Options



Options Dialog - General Sheet

This sheet lets you define various parameters depending on the type of plot. Lookup the plot you are interested in among the sections below:

- Line Plot
- 2D Scatter Plot
- 3D Scatter Plot

- Normal Probability Plot
- Histogram
- Matrix Plot
- Special plot “Percentiles”
- Special plot “Mean and SDev”
- Special plot “Predicted with Deviations”

Options Dialog - Sample Grouping Sheet

This sheet is available for sample oriented plots, i.e. 2D or 3D scatter plots and normal probability plots of samples, where the variables are model results (Results Viewer) or raw data (plotted from the Editor).

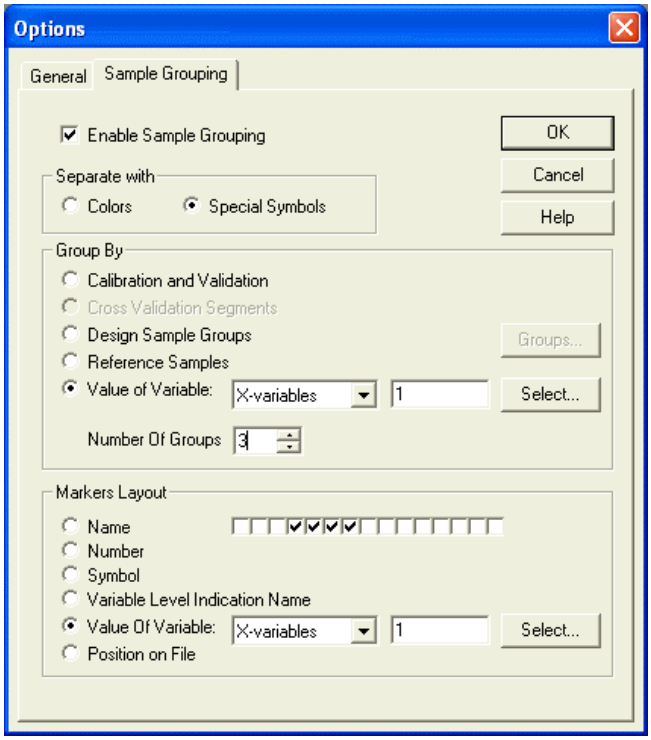
Examples:

- 2D score plot in PCA;
- 3D scatter plot of raw data;
- N-plot of Y-residuals in PLS.

Sample grouping makes predefined groups of samples appear more clearly on the plot, by means of colors or special symbols.

To start specifying your Sample Grouping options, check the box Enable Sample Grouping at the top of the dialog box, as shown below.

Dialog: Options - Sample Grouping sheet



In the field Separate with, you can choose to visually differentiate between groups of samples either with colors or with symbols. The Special Symbols option is especially useful when printing out plots in black and white.

The Group By field lets you define how the plotted points are to be divided into groups. The available options are presented in the table below.

Group By options for Sample Grouping

Options	Description
Calibration and Validation	Uses different symbols/colors to separate between calibration samples, validation samples and samples used for both calibration and validation
Cross Validation Segments	Uses different symbols/colors on each cross validation segment
Design Sample Groups	The groups correspond to the levels of one or several chosen design variables.
Reference Samples	Uses different symbols/colors to separate between the reference samples and the other samples.
Value of Variable	Samples with the same level in this variable get the same symbol/color. For continuous variables, up to 5 groups can be created.

If you take the option Design Sample Groups, the Groups… button is activated. Click this to access the **Sample Subgrouping** dialog, where you can select which design variable(s) must be used to generate the groups.

If you take the option Value of Variable, you need to specify which type of variable shall be used for the grouping: a Levelled variable, an X-variable or a Y-variable, from the drop-down list. Then you may either type in the variable number in the open text field, or click Select… to access the **Select Variable** dialog. This dialog is like a small editor, showing you the available variables among the chosen variable type, and letting you select one of these variables with the mouse.

In Number of Groups you may tune the number of groups to be generated with the help of the arrows (between 1 and 5 groups can be generated). The Number of Groups option is not available for Levelled variables; in this case, the number of groups is automatically defined as one group per level.

The field Markers Layout contains options available for the layout of the markers in plots. The available options are presented in the table below.

Markers layout options for Sample Grouping

Options	Description
Name	Take this option to display the sample names on the plot. Use the tick boxes to select the part of the name to be displayed in the plot.
Number	Take this option to display the sample numbers on the plot. The basis for the numbering is the current Set
Symbol	The data points are represented by a symbol, e.g. a small circle, which does not give any information about the point.
Variable Level Indication Name	The level of the sample is used to generate the marker, for example ++-+. This requires a designed data table
Position on file	The basis for the numbering is the raw data
Value of Variable	Use the value of a specific variable as marker for the samples. Category variables are useful with this option. Use the tick boxes to select the part of the level names to be displayed in the plot.

If you take the options Name or Value of Variable, use the tick boxes to select which part of the name, level name or numerical value shall be displayed on the plot.

The first mouse click on a character in the name string indicates the start of a character sequence. The next click indicates the end of the name string. All characters in between are selected. If you want to select characters that are not in sequence, hold down the <Ctrl> key when you select the characters you want in the label with the mouse. Deselect one by using <Ctrl> and clicking again.

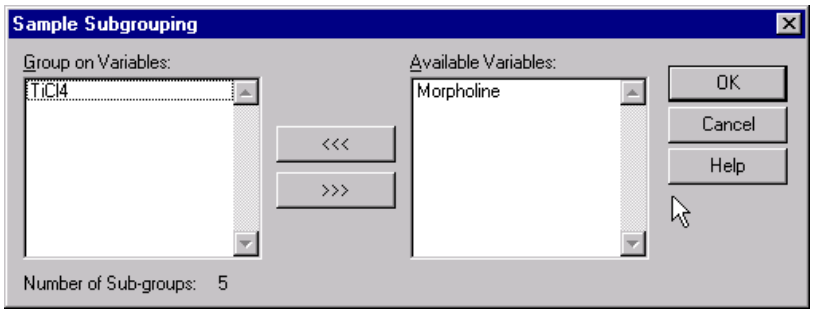
If you take the option Value of Variable, you need to specify which type of variable shall be used as a marker: a Levelled variable, an X-variable or a Y-variable, from the drop-down list. Then you may either type in the variable number in the open text field, or click Select… to access the **Select Variable** dialog. This dialog is like a small editor, showing you the available variables among the chosen variable type, and letting you select one of these variables with the mouse.

Note: The sample grouping information is more straightforward to read if you select the same variable in the Group By field as in the Markers Layout field. However, *grouping* by one variable and displaying the values of another variable as *markers* may be useful to include more information into a single plot.

Sample Subgrouping Dialog

In the **Sample Subgrouping** dialog, select which design variable(s) must be used to generate sample groups for the Sample Grouping display.

Dialog: Sample Subgrouping

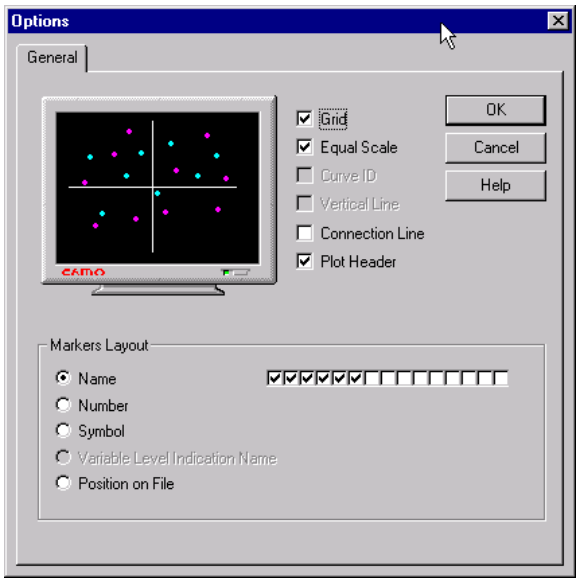


This dialog consists of two fields; Group on Variables and Available Variables. Select the variables you wish to use from the latter field and move them to the former using the appropriate arrow button. The number of sub-groups is displayed at the bottom of the dialog; the number depends on the variables' numbers of levels. Choosing one design variable with three levels, e.g., will give three sub-groups, while two such variables will give 3 x 3 = 9 sub-groups.

Options Dialog - General Sheet for 2D-, 3D Scatter And Normal Probability Plots

Accessed from **Edit - Options** for a 2D-scatter plot, 3D-scatter plot or Normal Probability plot, this sheet lets you define the plot layout.

Dialog: Options - General sheet for 2D-Scatter, 3D-Scatter or Normal Probability plot



Options in the General sheet apply to all the data points in the plot. The check boxes in the upper field are used to characterize the plots more closely and are enabled and disabled according to which type of plot is activated. The available boxes and their characteristics are listed below.

General options for 2D-Scatter, 3D-Scatter or Normal Probability plots

Option	Description
Grid	Displays a grid, allowing you to see the data points' coordinates more clearly.
Equal Scale	Applies equal scaling along all axes in the plot.
Curve ID	Identifies each curve in the plot with a name or number.
Vertical Line	Draws vertical lines from the data points to the horizontal plane in 3D scatter plots.
Connection Line	Draws a line between consecutive data points. This is useful to see the development when the data points are sorted.
Plot Header	Draws the title of the plot and axis names.

In the Markers Layout field, you choose how markers and labels will appear in the plot. Available options are given below.

Markers layout options

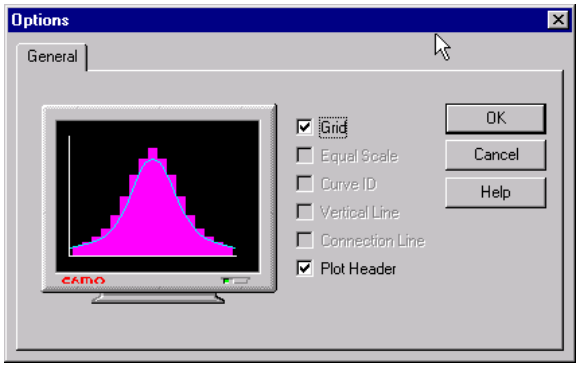
Options	Description
Name	Select which part of the name to use in the plot with the tick-boxes.
Number	The basis for the numbering is the current Set
Symbol	The data points are represented by a symbol, e.g. a small circle, which does not give any information about the point.
Variable Level Indication Name	The level of the sample is used to generate the marker, for example ++-+. This requires a designed data table
Position on file	The basis for the numbering is the raw data

To the right of the radio button Name, you choose which of the characters of the name you want to display. The first mouse click on a character in the name string indicates the start of a character sequence. The next click indicates the end of the name string. All characters in between are selected. If you want to select characters that are not in sequence, hold down the <Ctrl> key when you select the characters you want in the label with the mouse. Deselect one by using <Ctrl> and clicking again.

Options Dialog - General Sheet for Histograms

Accessed from Accessed from **Edit - Options** for a histogram, this sheet lets you define the plot layout.

Dialog: Options - General sheet for Histograms



Options in the General sheet apply to all the data points in the plot.

The check boxes in the upper field are used to closer characterize the plot, and are enabled and disabled according to which type of plot is activated. The options are listed below.

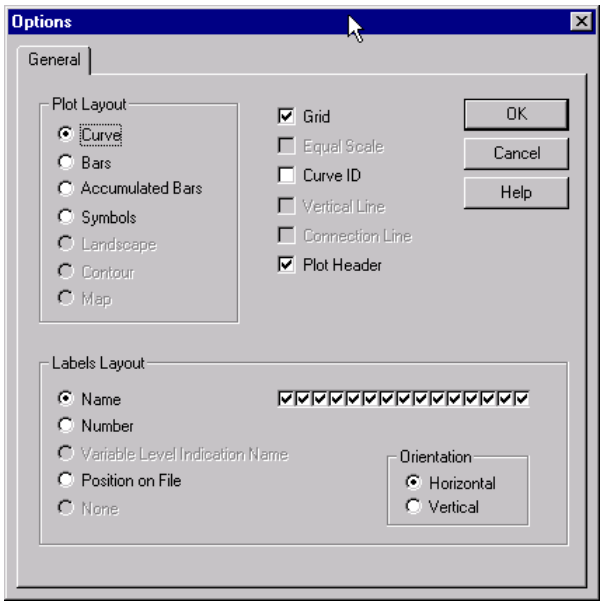
General plot options available for histograms

Option	Description
Grid	Displays a grid, allowing you to see the data points' coordinates more clearly.
Plot Header	Draws the title of the plot and axis names.

Options Dialog - General Sheet for Line and Matrix Plots

Accessed from **Edit - Options** for a Line plot or Matrix plot, this sheet lets you define the plot layout.

Dialog: Options - General sheet for Line plots and Matrix plots



Options on the General sheet apply to all the data points in the plot.

The check boxes in the upper right field are used to closer characterize the plots, and are enabled and disabled according to which type of plot is activated. The available boxes and their characteristics are listed below.

General plot options available for Line plots or Matrix plots

Option	Description
Grid	Displays a grid, allowing you to see the data points' coordinates more clearly.
Curve ID	Identifies each curve in the plot with a name or number.
Plot Header	Draws the title of the plot and axis names.

In the field Plot Layout you define how the plot is drawn. You select the type of plot you want by clicking on the appropriate radio button. The available options are described below. Note that not all radio buttons will be enabled in every plot.

Plot Layout options

Option	Description
Curve	Each object is plotted as a line
Bars	Each data point is plotted as a bar
Accumulated bars	The bars from different objects are put on top of each other in the same variable
Symbols	Each data point is a symbol only.
Landscape	The selected data is plotted as a landscape
Contour	The matrix is seen from above, and the contours indicate value levels
Map	The matrix is seen from above, using different colors to indicate different values

In the Labels Layout field, you choose how markers and labels will appear in the plot. Available options are given below.

Labels layout options

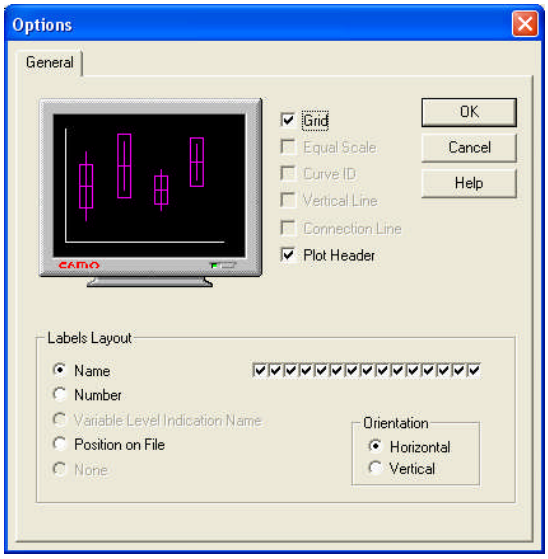
Options	Description
Name	Select which part of the name to use in the plot
Number	The basis for the numbering is the current Set
Variable Level Indication Name	The level of the sample is used to generate the name, for example ++-+. This requires a designed data table
Position on file	The basis for the numbering is the raw data
None	No label
Orientation field	Horizontal or Vertical

To the right of the radio button Name, you choose how you want to build up the name character string. The first mouse click on a character in the name string indicates the start of a character sequence. The next click indicates the end of the name string. All characters in between are selected. If you want to select characters that are not in sequence, hold down the <Ctrl> key when you select the characters you want in the label with the mouse. Deselect one by using <Ctrl> and clicking again.

Options Dialog - General Sheet for "Predicted with Deviations" and "Percentiles"

Accessed from **Edit - Options** for special plots “Predicted with Deviations” or “Percentiles”, this sheet lets you define the plot layout.

Dialog: Options - General sheet for “Predicted with Deviations” or “Percentiles”



Options on the General sheet apply to all the data points in the plot.

The check boxes in the upper right field are used to closer characterize the plots, and are enabled and disabled according to which type of plot is activated. The available boxes and their characteristics are listed below.

General plot options available for Predicted with Deviations or Percentiles

Option	Description
Grid	Displays a grid, allowing you to see the data points' coordinates more clearly.
Plot Header	Draws the title of the plot and axis names.

In the Labels Layout field, you choose how markers and labels will appear in the plot. Available options are given below.

Labels layout options

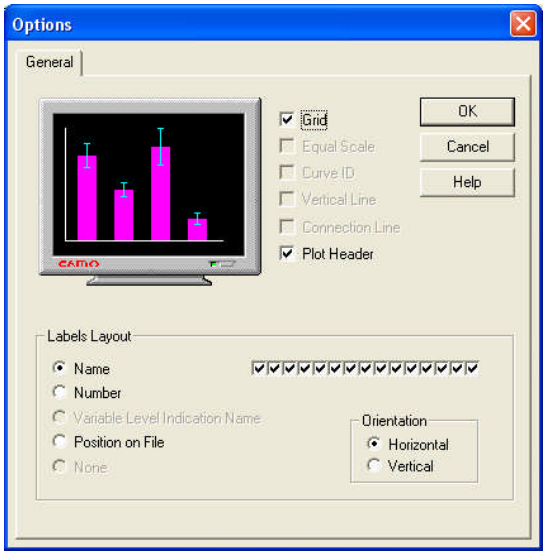
Options	Description
Name	Select which part of the name to use in the plot
Number	The basis for the numbering is the current Set
Variable Level Indication Name	The level of the sample is used to generate the name, for example ++-+. This requires a designed data table
Position on file	The basis for the numbering is the raw data
None	No label
Orientation field	Horizontal or Vertical

To the right of the radio button Name, you choose how you want to build up the name character string. The first mouse click on a character in the name string indicates the start of a character sequence. The next click indicates the end of the name string. All characters in between are selected. If you want to select characters that are not in sequence, hold down the <Ctrl> key when you select the characters you want in the label with the mouse. Deselect one by using <Ctrl> and clicking again.

Options Dialog - General Sheet for "Mean and SDev"

Accessed from **Edit - Options** for a special plot "Mean and SDev", this sheet lets you define the plot layout.

Dialog: Options - General sheet for Mean and SDev



Options on the General sheet apply to all the data points in the plot.

The check boxes in the upper right field are used to closer characterize the plots, and are enabled and disabled according to which type of plot is activated. The available boxes and their characteristics are listed below.

General plot options available for Mean and SDev

Option	Description
Grid	Displays a grid, allowing you to see the data points' coordinates more clearly.
Plot Header	Draws the title of the plot and axis names.

In the Labels Layout field, you choose how markers and labels will appear in the plot. Available options are given below.

Labels layout options

Options	Description
Name	Select which part of the name to use in the plot
Number	The basis for the numbering is the current Set
Variable Level Indication Name	The level of the sample is used to generate the name, for example ++-+. This requires a designed data table
Position on file	The basis for the numbering is the raw data
None	No label
Orientation field	Horizontal or Vertical

To the right of the radio button Name, you choose how you want to build up the name character string. The first mouse click on a character in the name string indicates the start of a character sequence. The next click indicates the end of the name string. All characters in between are selected. If you want to select characters that are not in sequence, hold down the <Ctrl> key when you select the characters you want in the label with the mouse. Deselect one by using <Ctrl> and clicking again.

Edit - Insert Draw Item

You can add a drawing to the plot using this option. It is possible to draw with two different shapes

- Line ;
- Text .

Change Item Properties once it is Drawn

Mark the item by pressing the <Alt> key and clicking with the left mouse button at the same time. You can then delete the drawing item or change its properties. The item can also be moved around the plot by dragging it (while the <Alt> key is pressed down).

Once the item is selected, use **Edit - Item Properties** to change its properties (style, font, color…).

A marked draw item can also be moved by using the arrow keys.

Edit - Insert Draw Item - Line

Allows you to draw a line on a plot.

Click at the point in the plot where you want the line to start and hold the left mouse button down as you draw the line.

The properties of the line can be changed at a later stage by marking the item (Press the <Alt> key and click on the line) and selecting **Edit - Item Properties**.

For details on the **Line Properties** dialog, lookup page 144.

Edit - Insert Draw Item - Text

Allows you to insert a text element into your plots.

Place the cursor at the location where you want the text to appear, click with the left mouse button. This takes you to the dialog **Text Properties**, where you select the properties of the text. Type the text in the Text field and click OK.

The text can be changed at a later stage by marking the text item (Press the <Alt> key and click on the text) and selecting **Edit - Item Properties**.

For details on the **Text Properties** dialog, lookup page 145.

Edit - Delete Item

The option is only enabled if you have marked a drawing item (line, text, etc.) in a plot by pressing the <Alt> key and clicking on the item with the left mouse button. The item can then be deleted by way of this menu choice.

Edit - Item Properties…

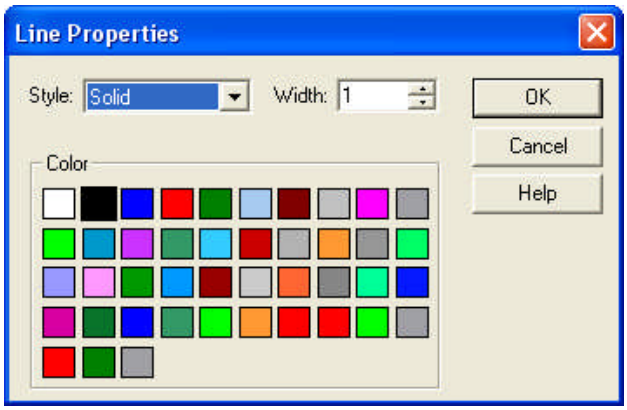
If you have marked a drawing item (line, text, etc.) in a plot by pressing the <Alt> key and clicking on the item with the left mouse button, the properties of the drawing item, such as style, width, and color, can be changed in the **Item Properties** dialog. The contents of the dialog depend on the type of draw item, see details below.

The dialog can also be reached by pressing the <Alt> key and double-clicking on the draw item with the left mouse button.

Line Properties Dialog

This dialog allows you to choose the properties of a line inserted in your plot as draw item.

Dialog: Line Properties



Make a choice from the Style drop-down list.

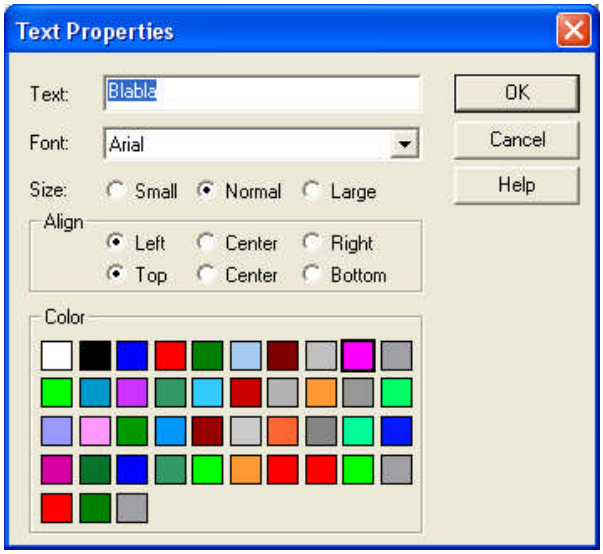
Tune Width up or down.

Select a suitable color (black is default) from the Color field.

Text Properties Dialog

This dialog allows you to choose the properties of a text inserted in your plot as draw item.

Dialog: Text Properties



Type in or correct your text in the Text field.

Make a choice from the Font drop-down list.

Make a choice of Size and horizontal / vertical alignment using the corresponding radio buttons.

Select a suitable color (black is default) from the Color field.

Edit - Mark

Mark objects (samples or variables) you want to focus on in your interpretation.

The menu option **Edit - Mark** has 8 sub-options:

- Outliers Only
- Test Samples Only
- Evenly Distributed Samples Only…
- Significant X-Variables Only
- With Rectangle
- One By One
- Reverse Marking
- Unmark All

Edit - Mark: Basic Notions

A typical use of this command is to mark extreme samples in a score plot and investigate the behavior of those samples on other plots. Another is to mark ranges of the spectra in the “Important variables” plot, to make a new model based on only important wavelengths.

Note: If your Viewer contains more than one plot, marking is only possible from the currently active sub-view. For instance, if the currently active sub-view contains a score plot, you have to click on the sub-view containing a variable plot before you can mark any variables.

Once you have marked objects, they appear marked in all current and future plots, until you unmark them or close the Viewer.

Edit - Mark - Outliers Only

All outliers found by The Unscrambler’s automatic outlier detection are marked. The limits used for detecting the outliers are set in the **Warning Limits** dialog. You access this dialog from all model dialogs.

Edit - Mark - Test Samples Only

or **Ctrl+T**

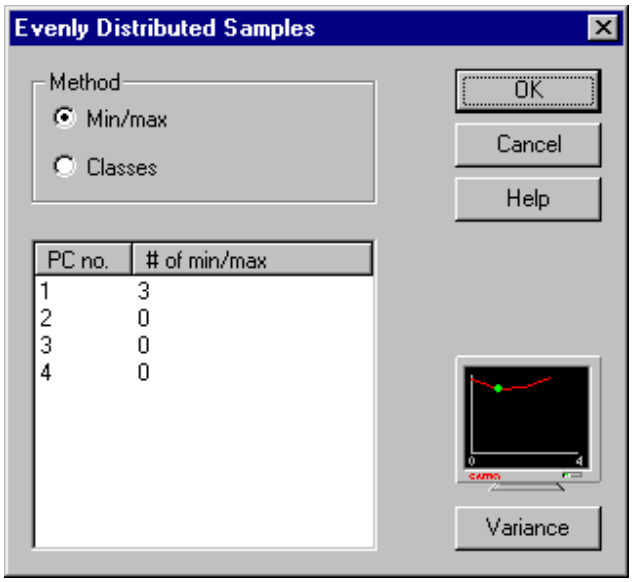
All test samples are marked. The option requires that the model used to create the plot is made using test set validation.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Edit - Mark - Evenly Distributed Samples Only…

This command lets you mark a representative subset of the samples in any plot of samples. You specify which samples to mark in the dialog **Evenly Distributed Samples**, which is displayed below.

Dialog: Evenly Distributed Samples



In the Methods field, choose whether you want to mark by Min/max or by Classes. Then, in the list below, specify the number of PCs (listed in the left column) for which you want to mark samples, and how many (listed in the right column). No samples are marked for PCs with 0 in the right column, i.e., in the above figure, only PC 1 is marked.

If you select the method Min/max, a number of extreme samples will be picked out for each PC, according to your specification in the right column in the list below the Methods field. It will be labeled # of Min/max, and for each Min/max selected, two extreme samples are marked (max and min value). Thus, setting the number to 3 will mark a total of six samples.

If you select the method Classes, the samples will be divided into a number of classes for each PC. One pair of extreme samples (max and min value) will be picked out for each PC, according to your specification in the right column in the list below the Methods field. It will be labeled # of Classes, and for each class, two extreme samples are marked. Thus, setting the number to 3 will mark a total of six samples.

If you wish to include variance, press the Variance button to launch the **Variance** dialog.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Edit - Mark - Significant X-Variables Only

This command is available if you have chosen the Uncertainty Test option in a multivariate regression model. When using this function, The Unscrambler can mark the significant X-Variables in the model describing Y.

The marking of significant X-variables is accessed either from the Edit menu **Edit - Mark Significant X-Variables only** or from the specific icon shown above. This marking applies simultaneously to all relevant

plots on screen: Loading, X-loading Weights and Y-loading and finally the Regression Coefficients plot. Marking is available for any kind of data.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Beware of misinterpretations with PLS 2!

In the case of PLS2 models, significant X-Variables may differ from one specific Y-Variable to the other. To avoid misinterpretation, the marking is removed when the user plots a new Regression Coefficients plot in another window. The un-marking is also performed when plotting Regression Coefficients for another Y-Variable. Make sure to click the **Mark Significant X-Variables** icon –again– while the Regression Coefficients plot you are studying is active!

Edit - Mark - With Rectangle

When this option is active, you can draw a rectangle in the plot. All objects within the rectangle are marked.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Edit - Mark - One By One

or **Ctrl+M**

Choose this option to use the mouse to mark objects one by one. A click on an already marked object unmarks it. Turn the marking mode off by clicking outside the active plot or with the right mouse button within the plot.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Edit - Mark - Unmark All

or **Ctrl+U**

All marked objects in the current plot are de-selected. The same objects are also unmarked in all other sub-views.

Note: If your Viewer contains more than one plot, “Unmark All” applies to objects displayed in the currently active sub-view. For instance, if you are viewing a score plot with marked samples, and a loading plot with marked variables, choosing “Unmark All” while the score plot is active will de-select the marked samples, but will not affect the marked variables.

Edit - Mark - Reverse Marking

Choose this option to reverse the current marking status on a plot. All unmarked objects/variables will become marked and all marked objects/variables will become unmarked in one click.

For more general information about marking, lookup section Edit - Mark: Basic Notions.

Edit - Copy All

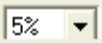
Copies all plots displayed in your Viewer (in the system of 2 or 4 sub-views) onto the clipboard. You may later on paste the contents of the clipboard into the target of your choice (Word, Excel…) and the copied plots will appear with the same layout as they had in the Viewer.

Edit - Select Bars…

Select how many bars are to be used in histogram plots. The Unscrambler calculates the value limits for each bar. The number of bars must lie within the limits given in brackets.

Adding more bars gives you more details about the distribution of the data points.

Choose Significance Level



This command is accessed from the toolbar only when viewing classification results. The tool is active for the following plots:

- Classification table
- Cooman's plot
- Si vs Hi
- Si/S0 vs Hi

Choose the desired significance level (either "None" or between 0.1% and 25%) for the classification results, by clicking on the arrow and selecting desired level from the list.

If you tune up the significance level (e.g. from 5% to 10%) this will narrow down the class limits (more samples are rejected).

If you tune it down (e.g. from 5% to 1%) this will widen up the class limits (fewer samples are rejected).

If you choose "None" on the Cooman's plot, Si vs Hi or Si/S0 vs Hi, this will remove any significance limits form the plot.

Significance Limits = None

In the case of 2-D scatter plots (Cooman's plot, Si vs Hi, Si/S0 vs Hi), an additional level is available. Select "None" from the drop-down list if you wish to display the plot ***without any significance limits***.

The View Menu

View - Sample Statistics

Displays a few descriptive statistics about your samples in a new Editor. You first access the **Sample Statistics** dialog, where you must select a Variable set.

The computed statistics are:

- Number of missing values;
- Minimum;
- Maximum;
- Mean;
- Standard deviation;
- Skewness.

The results are displayed in a new Editor. This new Editor behaves as a "slave" of the source data Editor. As a consequence, rows marked in the original data table will also be marked in the Sample Statistics table, and vice versa.

An example of Sample Statistics results

		#of Missing	Min	Max	Mean	SDev	Skewness
		1	2	3	4	5	6
Calibration	1	0.0000	2.0000	10.0000	7.3333	4.6188	–0.3849
Calibration	2	0.0000	4.0000	20.0000	14.6667	9.2376	–0.3849
Calibration	3	0.0000	10.0000	32.0000	19.3333	11.3725	0.2679
Calibration	4	0.0000	20.0000	44.0000	30.6667	12.2202	0.2078
Calibration	5	0.0000	0.0000	0.0000	0.0000	0.0000	m
Calibration	6	0.0000	3.0000	15.0000	11.0000	6.9282	–0.3849
Calibration	7	0.0000	5.0000	31.0000	15.6667	13.6137	0.3025
Unknown	8	1.0000	12.0000	21.6000	16.8000	6.7882	2.0722e–07
Unknown	9	1.0000	20.0000	42.4000	31.2000	15.8392	–7.2497e–09
Unknown	10	1.0000	13.2000	18.0000	15.6000	3.3941	–2.0722e–07

The usual **File**, **Edit**, **View**, **Modify** and **Task** operations are not allowed on this slave Editor; only **Plot** is possible. Besides, closing the Editor containing the source data table will also close the Sample Statistics table.

If you want to manipulate these statistics further, you have to select rows or columns of the Sample Statistics table, and drag'n drop them onto an empty spot of the workplace. This will generate a new table which you can freely manipulate, edit and save.

View - Sample Statistics (3-D)

This option is disabled for all 3-D data tables, no matter which layout they have.

Useful tips

1- To display Sample Statistics for an O^2V table, select the whole table then drag and drop it unto an empty spot of the workspace (alternatively use **File - Duplicate - As 2-D Data Table**). You may then display Sample Statistics on the resulting 2-D table.

2- To display Sample Statistics for an OV^2 table, two solutions are possible.

Duplicating the table as 2-D and displaying Sample Statistics will give you a summary where Primary and Secondary variables are taken into account together.

If you are interested in Sample Statistics across individual Primary (resp. Secondary) variables, here is what you can do. Select the sample you want to focus on. Choose **File - Convert Vector to Data Table**. The resulting 2-D table has as many rows as you had Secondary variables, and as many columns as you had Primary variables. Display Sample Statistics on that table if you want a summary of each Secondary variable across all Primary variables. Display Variable statistics if you want a summary of each Primary variable across all Secondary variables.

View - Variable Statistics

Displays a few descriptive statistics about your variables in a new Editor. You first access the **Variable Statistics** dialog, where you must select a Sample set.

The computed statistics are:

- Number of missing values;
- Minimum;
- Maximum;
- Mean;
- Standard deviation;
- Skewness.

The results are displayed in a new Editor. This new Editor behaves as a “slave” of the source data Editor. As a consequence, columns marked in the original data table will also be marked in the Variable Statistics table, and vice versa.

An example of Variable Statistics results

		Red	Blue	Comp "a"
		1	2	3
#of Missing	1	0.0000	0.0000	3.0000
Min	2	0.0000	0.0000	0.0000
Max	3	28.0000	44.0000	20.0000
Mean	4	15.0000	19.3200	11.4286
SDev	5	7.4833	17.1786	7.4801
Skewness	6	–0.2663	0.2050	–0.1567

The usual **File**, **Edit**, **View**, **Modify** and **Task** operations are not allowed on this slave Editor; only **Plot** is possible. Besides, closing the Editor containing the source data table will also close the Variable Statistics table.

If you want to manipulate these statistics further, you have to select rows or columns of the Variable Statistics table, and drag’n drop them onto an empty spot of the workplace. This will generate a new table which you can freely manipulate, edit and save.

View - Variable Statistics (3-D)

This option is disabled for all 3-D data tables, no matter which layout they have.

Useful tips

1- To display Variable Statistics for an OV^2 table, select the whole table then drag and drop it unto an empty spot of the workspace (alternatively use **File - Duplicate - As 2-D Data Table**). You may then display Variable Statistics on the resulting 2-D table.

2- To display Variable Statistics for an O^2V table, two solutions are possible.

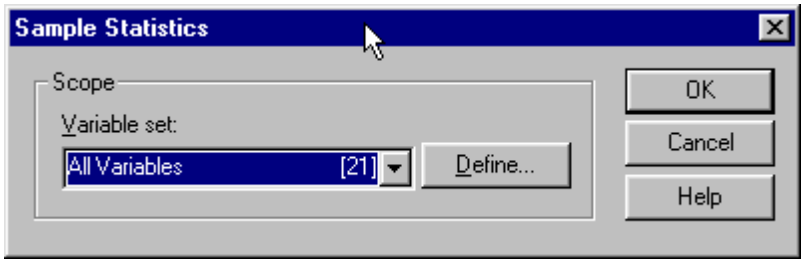
Duplicating the table as 2-D and displaying Variable Statistics will give you a summary where Primary and Secondary samples are taken into account together.

If you are interested in Variable Statistics across individual Primary (resp. Secondary) samples, here is what you can do. Select the variable you want to focus on. Choose **File - Convert Vector to Data Table**. The resulting 2-D table has as many rows as you had Primary samples, and as many columns as you had Secondary samples. Display Variable Statistics on that table if you want a summary of each Secondary sample across all Primary samples. Display Sample statistics if you want a summary of each Primary sample across all Secondary samples.

Sample Statistics Dialog and Variable Statistics Dialog

The dialogs **Sample Statistics** and **Variable Statistics** let you compute simple statistics for all samples or variables in your data table.

Dialog: Sample Statistics



In the field Scope you select the Variable set (for Sample Statistics) or Sample set (for Variable Statistics) on which the statistics will be based.

For example, if you have chosen **View - Sample Statistics**, you will access the **Sample Statistics** dialog where you can select Variable set "Sensory descriptors"; the statistics will be displayed as a table with ***all your samples*** as rows, and the ***minimum, maximum, etc***. over the ***Sensory descriptors*** as columns.

If necessary, use the Define… button to access the **Set Editor** dialog and define a new variable set.

The results will be displayed in a new Editor, which behaves as a "slave" of the source data Editor.

For more details, see:

- The View Menu
- View - Sample Statistics
- View - Variable Statistics

View - Sample Names

This option shows the design sample names for designed data tables in the Editor.

View - Point Names

Applies to designed data only, and shows a string of + and - characters according to the variable levels of the samples in the Editor. Variables with several levels are indicated by the level number instead.

View - X/Y Variable Numbering

Replaces the column numbers in the Editor with an identifier so that you can see which columns belong to the X-matrix and Y-matrix respectively, and which level variables you have.

This option is only available when you start the Editor from a result plot in the Viewer using **View - Raw Data**.

View - Level Indices

Replaces the level names with level indices (0,1,2,…) in all levelled variables (Category or Design variables).

This option is only available when the currently active table contains at least one levelled variable.

View - Standard Sample Sequence

This option only applies to designed data. If you activate the option, samples in the Editor are shown according to the standard design order. Use this option to see the logic of the design.

View - Experiment Sample Sequence

This option only applies to designed data. Through this option, samples in the Editor are shown in randomized order, i.e. in the same sequence as the experiments are supposed to be performed.

View - Graphical

Lets you view the selected data of a Viewer in graphical mode. Use this command to return to a graphical view after examining your results as a numerical table (**View - Numerical**).

View - Numerical

Through this option you may display results plotted in a Viewer as a numerical table. You can copy that data table to the Clipboard and paste it into an Editor or another software package.

Restore the plot using **View - Graphical** or **Ctrl+G**.

View - Autoscale

or **Ctrl+H**

Scales the plot so that all data points are shown within the Viewer window. This command is useful after you have used **Add Plot** and **Scaling**.

View - Scaling

You can change the plot by scaling its axes to fit the range you want. You may scale the plot in 4 ways:

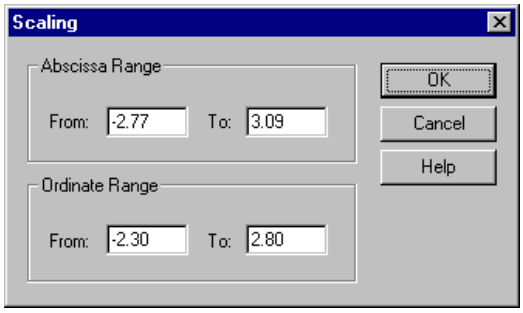
1. Select the minimum and maximum values on each axis: Min/Max Scaling;
2. Use a frame to select the desired plot range: Frame Scaling;
3. Select the exact min. and max. values on each axis: Exact Min/Max Scaling;
4. Use an exact frame: Exact frame Scaling.

Use **Autoscale** to display the plot as it was originally.

View - Scaling - Min/Max

You enter the dialog **Scaling**, where you must specify which area of the plot to display. You may specify values that are outside the current ranges.

Dialog: Scaling



The Unscrambler actually adjusts the plot range to make it look nice when you use this option. Use the command **Exact Min/Max** if you need higher precision in your scaling.

In the field Abscissa Range, you enter the minimum and maximum axis value for the horizontal axis. Then, you enter the minimum and maximum axis value for vertical axis in the field Ordinate Range and click OK.

View - Scaling - Frame

With this command you can select a sub-rectangle of the current plot with a frame. The selected region is then blown up to fill the entire plot area.

The Unscrambler actually adjusts the plot range to make it look nice when you use this option. Use the command **Exact Frame** if you need higher precision in your scaling.

View - Scaling - Exact Min/Max

Specify which area of the plot to display. You may specify values that are outside the current ranges. The Unscrambler does not adjust the scaling to make the plot look nice when this command is used. If you want the axes and grid to look nicer, try the command **Min/Max Scaling** instead.

The scaling is done in the **Exact Scaling** dialog. In the field Abscissa Range, you enter the minimum and maximum axis value for the horizontal axis. Then, you enter the minimum and maximum axis value for vertical axis in the field Ordinate Range and click OK.

View - Scaling - Exact Frame

Select a sub-rectangle of the current plot with a frame. The selected region is then blown up to fill the entire plot area.

The Unscrambler does not adjust the scaling to make the plot look nice when this command is used. If you want the axes and grid to look nicer, try the command **Frame Scaling** instead.

View - Zoom In

Changes the plot scaling upwards in discrete steps, allowing you to view a smaller part of the original plot at a larger scale.

View - Zoom Out

This option scales the plot down by zooming out on the middle of the plot, so that you can see more of the plot, but at a smaller scale.

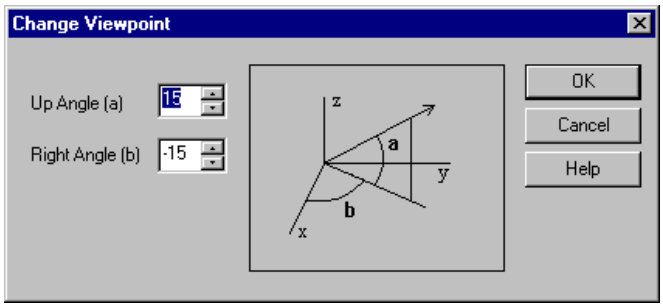
View - Viewpoint

You can set a specific viewpoint for 3D plots with the **Viewpoint - Change** command. Restore the original viewpoint using the **Viewpoint - Reset** command.

View - Viewpoint - Change

The viewpoint is changed in the **Change Viewpoint** dialog. In the Up Angle (a) field you enter the angle (in degrees) from which you want to view the plot in the vertical direction. 0 degrees is the XY plane. Then, you enter the angle from which you want to view the plot in the horizontal direction in the field Right Angle (b). 0 degrees is along the XZ plane.

Dialog: Change Viewpoint



You may return to the original viewpoint with the **Viewpoint - Reset** command.

View - Viewpoint - Reset

Use this command to return to the original viewpoint after you have changed the viewpoint using the **Viewpoint - Change** command.

View - Rotate

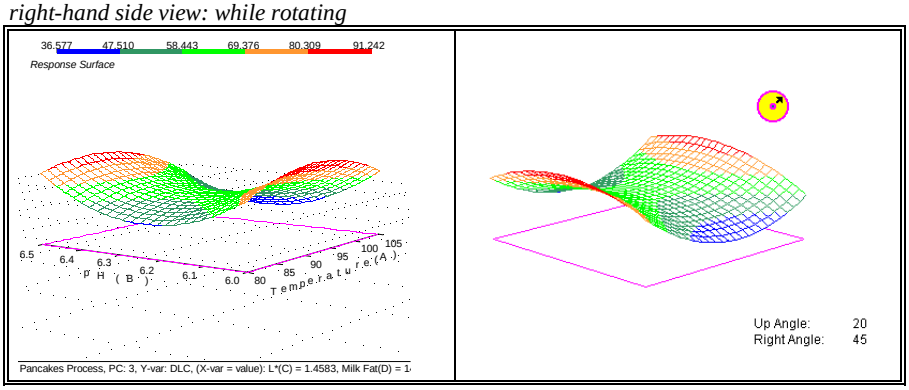
This function allows you to rotate **landscape response surface plots** and any other **3-D plot**. Use this feature in order to:

- get a better overview of the general shape of your response surface (see figure below),
- study the spatial distribution of your variables and samples. You can easily spot groups, outliers, or even errors in your data.

This function is accessed from the viewer menu **View - Rotate** or from the specific icon shown above.

Use either the left mouse button or the keyboard arrows to perform the rotation. This function provides a vertical rotation of 90° (↑ and ↓ arrows), and a horizontal rotation of 360° (← and → arrows). The rotation is executed 5° by 5° vertically and 10° by 10° horizontally. If you want a lower rotation or a view from a specific angle, you can rotate your response surface 1° by 1° by pressing the **Ctrl** key at the same time as the arrows.

Rotate Function used on a Response Surface plot (Landscape layout) - Left-hand side view: before or after the rotation, right-hand side view: while rotating



End the rotate function by clicking on the left mouse button anywhere outside the plot view.

Note: The menu option **View - Rotate** is available for all 3-D plots, regardless of the type of data plotted. This includes 3-D Scatter plots, and matrix plots in the bars and landscape layouts.

View - Projected

This command makes a quadruple plot from a 3D scatter plot. The upper right window shows the original 3D scatter plot. The other windows show the three different 2D scatter projections of the original 3D plot.

View - Plot ID

When this option is checked, a text line is included at the bottom of the plot with short-form plot details. Each curve ID is shown in the same color as the corresponding curve in the plot. The ID format varies according to the type of plot. The information given in the Plot ID field together with the Plot Identification window (**Window - Identification**) tells you all about the data displayed in the active plot.

To remove the text line, uncheck the option.

View - Plot Statistics

Makes a list of statistics pop up in the plot. Select this option again to remove the statistics from the plot.

This option is available for two types of plots only: 2D scatter plots and histograms. Which statistics are displayed depends on which plot you are in. An overview of which options are available in which situations is displayed below.

Available plot statistics in various contexts

Statistic	Interpretation	2D scatter plot	Histogram
Elements	Number of points	X	X
Slope	Slope of the regression line between X (abscissa) and Y (ordinate)	X	
Offset	Intercept of the regression line	X	
Correlation	Correlation between X and Y	X	
RMSEP	Root Mean Square Error of Prediction	X (Validation)	
RMSEC	Root Mean Square Error of Calibration	X (Calibration)	
RMSED	Root Mean Square Error of Deviations	X (other)	
SEP	Standard Error of Prediction	X (Validation)	
SEC	Standard Error of Calibration	X (Calibration)	
SED	Standard Error of Deviations	X (other)	

Bias	Average difference between Y and X	X	
Skewness	Asymmetry		X
Kurtosis	Flatness		X
Mean	Average value		X
Variance	Mean square of the deviations from the average		X
Sdev	Standard deviation: spread around the average		X

View - Trend Lines

Trend lines help you to interpret 2D scatter plots. You can plot two different trend lines:

5. regression line;
6. target line.

View - Trend Lines - Regression Line

or **Ctrl+E**

A regression line is drawn between the data points of a 2D scatter plot, using the least squares algorithm.

View - Trend Lines - Target Line

Inserts a target line in your 2D scatter plot.

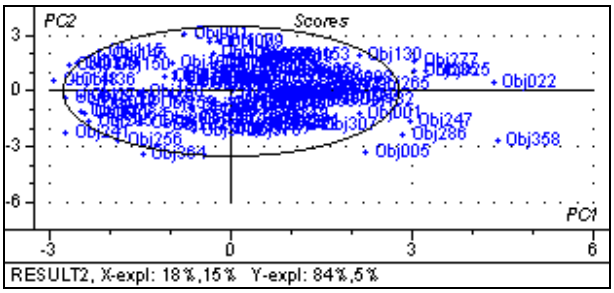
The target line is the line with slope = 1.0 and offset = 0.0 (or equation Y=X). In many cases this line will be the optimal solution, eg. in predicted vs. measured plots.

View - Hotelling T2 Ellipse

This function can be used whenever you have a Score plot available in a 2D Scatter plot layout.

The 95% confidence ellipse is based on Hotelling T^2 statistics. Observations found outside the ellipse are (potential) outliers. Note that in a normal situation you would expect about 5% of the samples to lie outside the ellipse.

Score plot with the Hotelling Ellipse.



View - Uncertainty Test

This command is available if you have chosen the Uncertainty Test option when performing a PCA or regression analysis.

It includes two options:

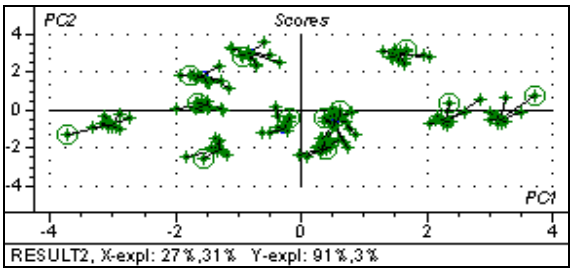
1. Stability Plot;
2. Uncertainty Limits.

View - Uncertainty Test - Stability Plot

Use this feature in order to visualize the stability of the model by showing perturbations around the main model. This will also indicate whether your uncertainty in Y is larger than in X.

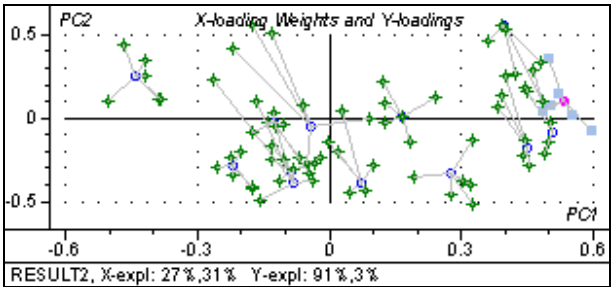
This function is accessed from the viewer menu **View - Uncertainty Test - Stability Plot** or from the specific icon shown above. This function can be applied when you are in any of the following 2-D scatter plots: Score, Loadings or X-loading Weights and Y-loadings. They are available for PCA, PCR and PLS models.

Score plot showing Jack-knife segments (Stability Plot)



The ***circle*** in the score plot corresponds to the rotated score for a given sample, for the segment where this sample was omitted from the model. It is useful to interpret the influence of this sample (see figure above).

X-loading Weights and Y-loadings Plot showing Stability results



The ***spread around each variable*** gives information about the ***stability*** of the model and each particular variable. Variables close to the origin often have larger spreads (which is an indication that they are not significant). When a variable has some extreme perturbation, it could be due to the fact that this variable has a skewed distribution. The individual Uncertainty Test values for the parameters can be imported from the result file. These are also stored for PCA, but the plotting options are not implemented.

When you have activated a stability plot, you can click on ***individual*** Jack-knifing points and a segment number will be displayed. This information will help you in finding out which samples are causing the variation.

View - Uncertainty Test - Uncertainty Limits

This command is available when a Regression Coefficients plot is currently active, in a Regression result generated with the option “Uncertainty Test”.

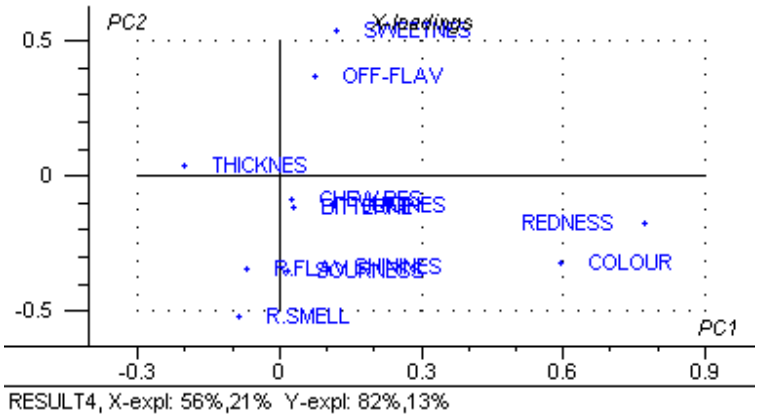
The limits are given as ± twice the estimated standard deviation for the coefficients (under ideal conditions this corresponds to approximately 95% confidence interval).

View - Correlation Loadings

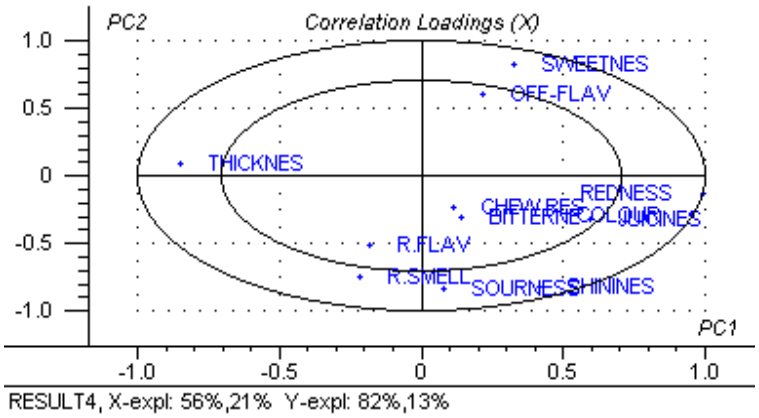
When a PCA, PLS or PCR analysis has been performed and a loading plot is displayed on your screen, use **View - Correlation Loadings** to take into account the amount of explained variance in your interpretation. The correlation loading plot will help you discover the structure in the data more clearly.

Below is a comparison between the ordinary Loadings plot and the Correlation Loadings plot. The importance of individual variables is visualized more clearly in the correlation loading plot compared to the standard loading plot. As an example, in the figures below, the importance of the sensory property Thickness becomes much more obvious when the correlation loadings ellipse is shown.

Usual Loading plot



Correlation Loading plot, displaying the two ellipses



Correlation loadings are computed for each variable for the displayed Principal Components. In the figure above, the outer ellipse is the unit-circle and indicates 100% explained variance. The inner ellipse indicates 50% of explained variance.

For information on the calculation of correlation loadings, we refer to Westad, 1999 (see chapter Bibliographical References).

Note: The Correlation Loadings plot can only be displayed if the currently active plot is a two-vector Loading plot. It does not apply to a plot of X-Loading Weights and Y-Loadings, nor to a line plot or a three-vector plot of Loadings.

View - Source

The toggle switches in this option give you an easy way to change the source data for the current plot, without going through the **Plot** menu. For instance, you can display Calibration variances only, Validation variances only, or both.

There are 13 options. How many of them are enabled depends on the kind of plot you are in. The options enabled in each type of plot are listed below.

Available sources in different plots

Option	Relevant Plot
Calibration	Sample plots, Variances
Validation	Sample plots, Variances
Previous Vertical PC	PC-dependent results
Next Vertical PC	PC-dependent results
Back to Suggested PC	PC-dependent results
Previous Horizontal PC	PC-dependent results
Next Horizontal PC	PC-dependent results
X-Variables	Variable plots, Variances
X1-Variables	Variable plots, Variances (Three-way PLS results)
X2-Variables	Variable plots, Variances (Three-way PLS results)
Y-Variables	Variable plots, Variances
Explained Variance	Variances
Residual Variance	Variances

Y-Residuals	Residuals
Studentized Residuals	Residuals

View - Source - Calibration

Shows or hides the calibration samples. This option can be combined with **Source - Validation** to see whether the calibration and validation results are similar. This option is only available in plots based on samples. You cannot disable both calibration and validation samples.

View - Source - Validation

Shows or hides the validation samples. This option can be combined with **Source - Calibration** to see whether the calibration and validation results are similar. This option is only available in plots based on samples. You cannot disable both calibration and validation samples.

View - Source - Previous Vertical PC

The command **View - Source - Previous Vertical PC** and its button "Previous Vertical PC" is part of the PC navigation tool. It allows you to switch to the previous PC along the vertical axis of the active plot.

Note:

You may also use the <arrow down> key as keyboard shortcut for this command.

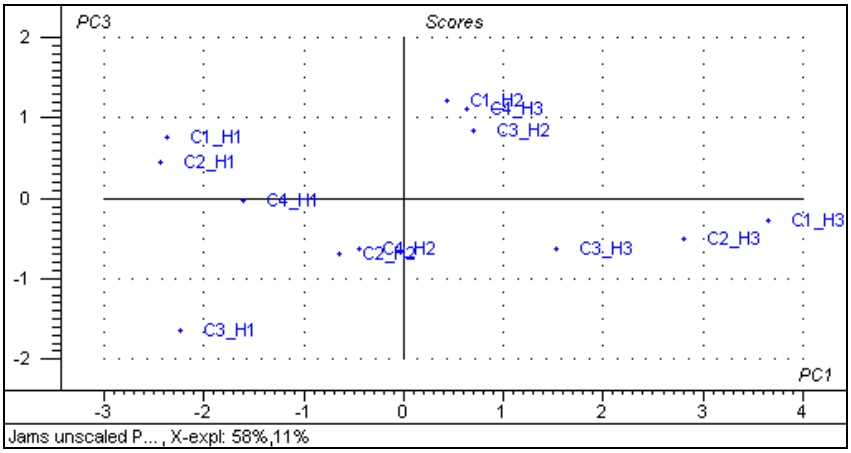
The command is available in the Viewer for PCA, PCR, MCR, PLS1, PLS2 and three-way PLS results, on 2D Scatter plots where the axes are Principal Components (or PLS components).

Note:

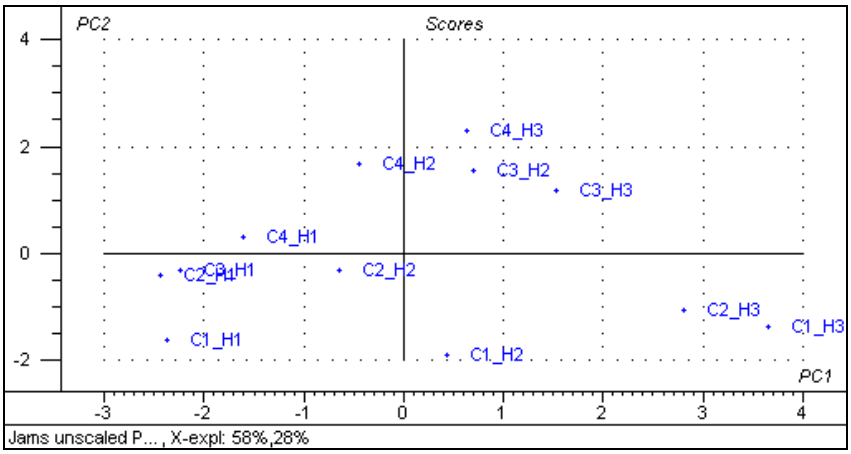
The command is not available for Line plots or 3D Scatter plots.

Example:

Scores plot from a PCA model, displayed for dimensions PC1 against PC3



After using the **Previous Vertical PC** button, the scores plot is displayed for dimensions PC1 against PC2



See also **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC**.

Note:

To access the **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC** buttons, activate the **Source** toolbar (**View - Toolbars...**)

View - Source - Next Vertical PC

The command **View - Source - Next Vertical PC** and its button "Next Vertical PC" is part of the PC navigation tool. It allows you to switch to the next PC along the vertical axis of the active plot.

Note:

You may also use the <arrow up> key as keyboard shortcut for this command.

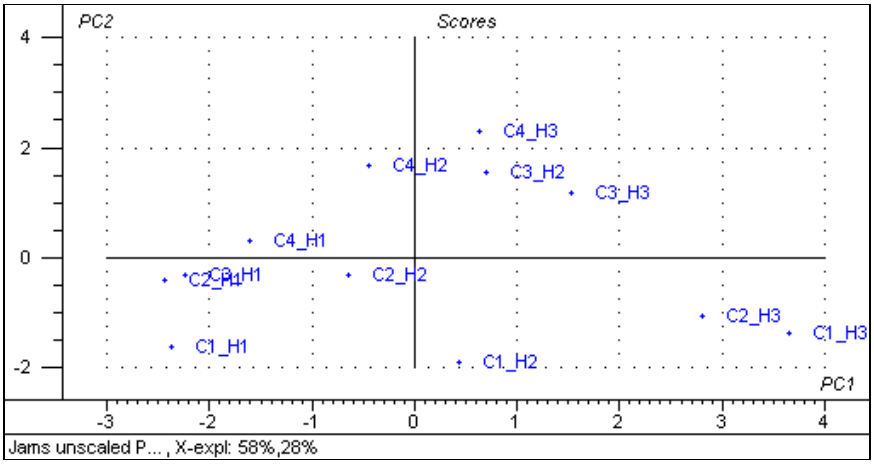
The command is available in the Viewer for PCA, PCR, MCR, PLS1, PLS2 and three-way PLS results, on 2D Scatter plots where the axes are Principal Components (or PLS components).

Note:

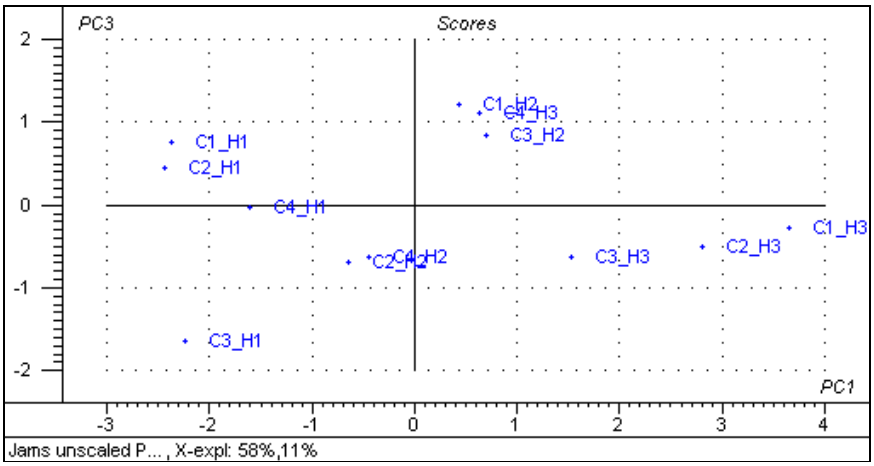
The command is not available for Line plots or 3D Scatter plots.

Example:

Scores plot from a PCA model, displayed for dimensions PC1 against PC2



After using the **Next Vertical PC** button, the scores plot is displayed for dimensions PC1 against PC3.



See also **Previous Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC**.

Note:

To access the **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC** buttons, activate the **Source** toolbar (**View - Toolbars...**)

View - Source - Back to Suggested PC

The command **View - Source - Back to Suggested PC** and its button "Back to Suggested PC" is part of the PC navigation tool. It allows you to switch back to the original axes after navigating with the "Previous…" and "Next…" options.

Note:

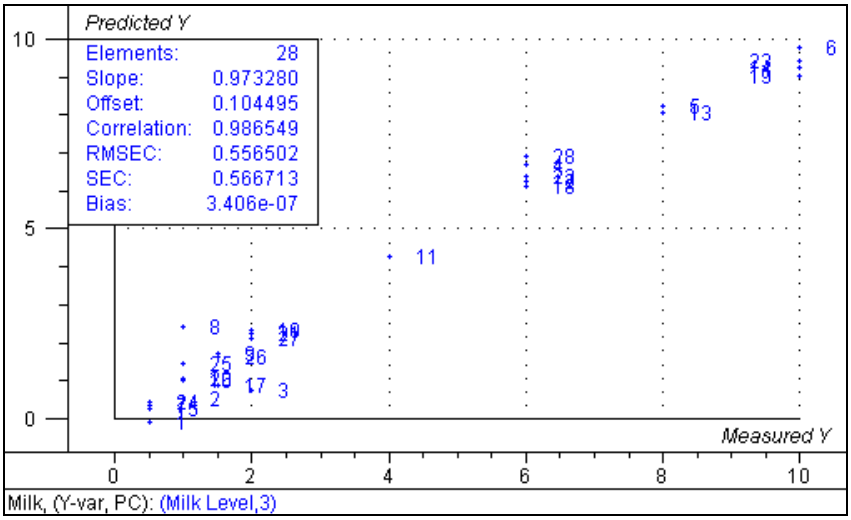
You may also use the <*> key as keyboard shortcut for this command.

In practice, here is what happens depending on the type of plot which is currently active:

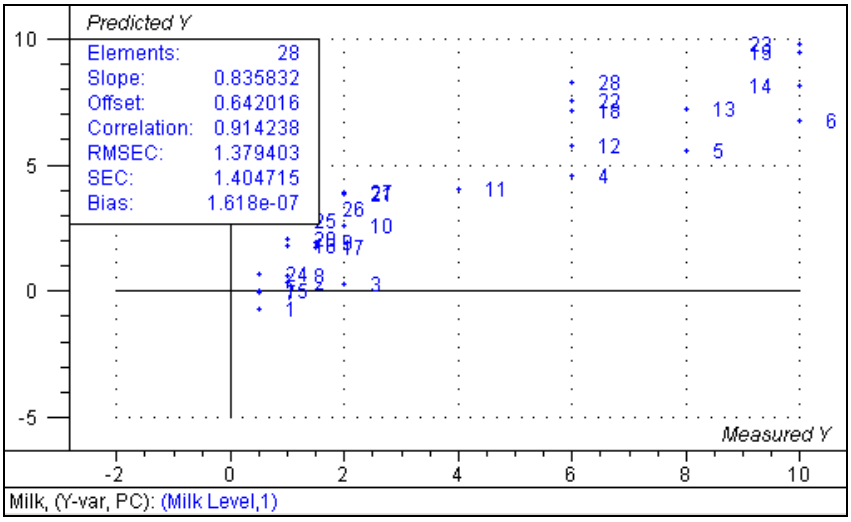
- On a 2D Scatter plot where the axes are Principal Components (or PLS components), e.g. Scores, Loadings or similar: go back to (PC1, PC2).
- On a line plot or 2D Scatter plot displayed for a specific number of PCs, e.g. Influence plot, Regression coefficients, Predicted vs Measured or similar: go back to the number of PCs suggested as optimal by the system.

Example:

Predicted vs. Measured plot from a PLS regression model, displayed for a model with three latent variables (PCs).



After using the **Back to Suggested PC** button, the Predicted vs. Measured plot is displayed for a model with one PC.



See also **Previous Vertical PC**, **Next Vertical PC**, **Previous Horizontal PC** and **Next Horizontal PC**.

Note:

To access the **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC** buttons, activate the **Source** toolbar (**View - Toolbars…**)

View - Source - Previous Horizontal PC

The command **View - Source - Previous Horizontal PC** and its button "Previous Horizontal PC" is part of the PC navigation tool. It allows you to switch to the previous PC along the horizontal axis of the active plot.

Note:

You may also use the <arrow left> key as keyboard shortcut for this command.

The command is available in the Viewer for PCA, PCR, MCR, PLS1, PLS2 and three-way PLS results, on plots of the following types:

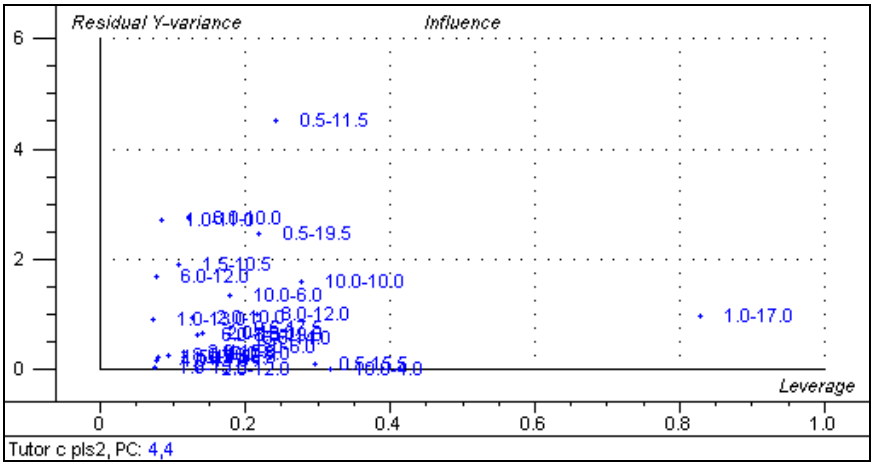
- 2D Scatter plots where the axes are Principal Components (or PLS components) e.g. Scores, Loadings or similar;
- Line plot or 2D Scatter plot displayed for a specific number of PCs, e.g. Influence plot, Regression coefficients, Predicted vs Measured or similar.

Note:

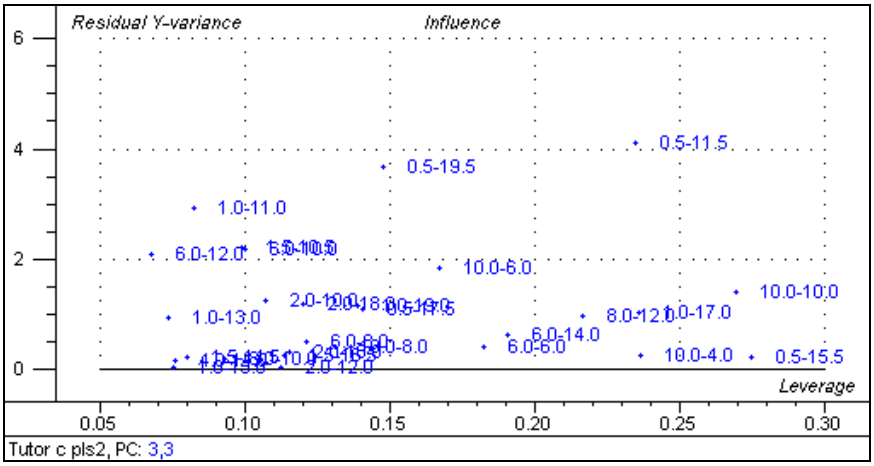
The command is not available for 3D Scatter plots.

Example:

Influence plot from a PLS regression model, displayed for a model with ***four*** latent variables (PCs).



After using the **Previous Horizontal PC** button, the Influence plot is displayed for a model with ***three*** PCs. Note that, in the present case, the Number of PCs is changed for the horizontal and vertical axes ***together*** (another combination would not make any sense).



See also **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC** and **Next Horizontal PC**.

Note:

To access the **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC** buttons, activate the **Source** toolbar (**View - Toolbars…**)

View - Source - Next Horizontal PC

The command **View - Source - Next Horizontal PC** and its button "Next Horizontal PC" is part of the PC navigation tool. It allows you to switch to the next PC along the horizontal axis of the active plot.

Note:

You may also use the <arrow right> key as keyboard shortcut for this command.

The command is available in the Viewer for PCA, PCR, MCR, PLS1, PLS2 and three-way PLS results, on plots of the following types:

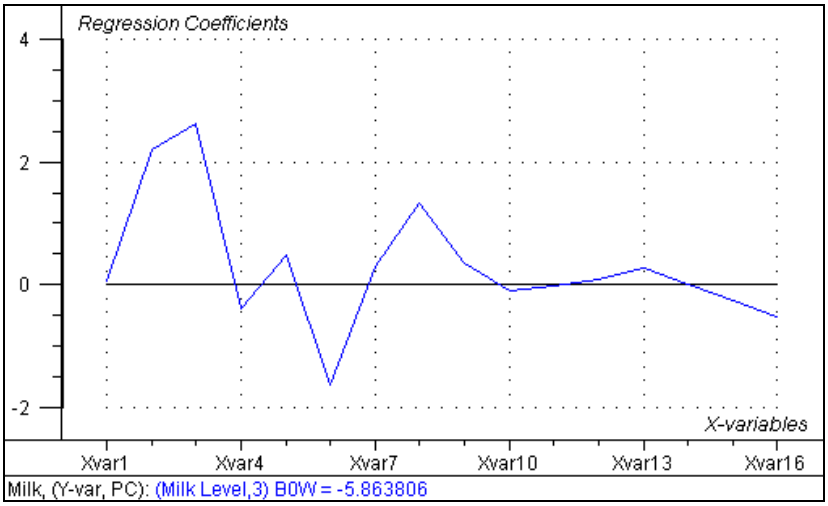
- 2D Scatter plots where the axes are Principal Components (or PLS components) e.g. Scores, Loadings or similar;
- Line plot or 2D Scatter plot displayed for a specific number of PCs, e.g. Influence plot, Regression coefficients, Predicted vs Measured or similar.

Note:

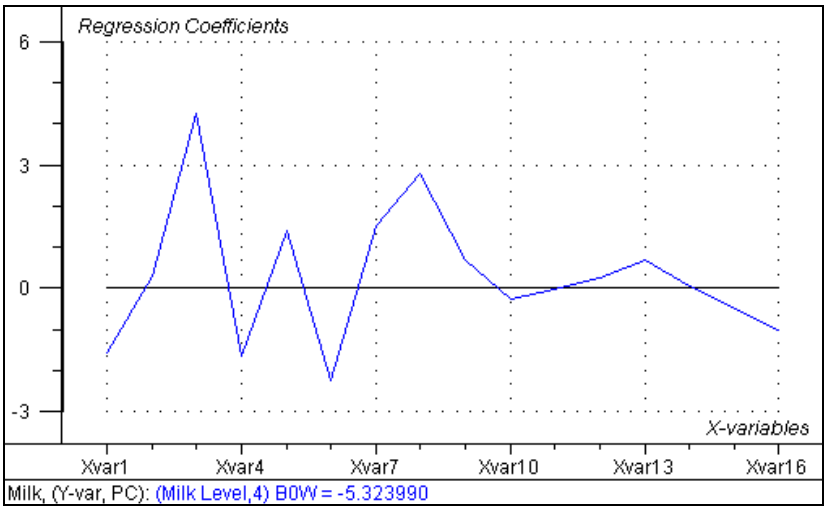
The command is not available for 3D Scatter plots.

Example:

Regression Coefficients plot from a PLS regression model, displayed for a model with three latent variables (PCs).



After using the **Next Horizontal PC** button, the Regression Coefficients plot is displayed for a model with four PCs.



See also **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC** and **Previous Horizontal PC**.

Note:

To access the **Previous Vertical PC**, **Next Vertical PC**, **Back to Suggested PC**, **Previous Horizontal PC** and **Next Horizontal PC** buttons, activate the **Source** toolbar (**View - Toolbars…**)

View - Source - X-Variables

Shows or hides the X-variables in a plot based on variables. This option is used in connection with loadings, variances, and variable plots. You cannot disable both X- and Y-variables.

View - Source - X1-Variables

Shows or hides the X1-variables (Primary X-variables) in a three-way PLS result plot based on variables. This option is used in connection with loading weights, variances, and variable plots. You cannot disable X1-, X2- and Y-variables simultaneously.

View - Source - X2-Variables

Shows or hides the X2-variables (Secondary X-variables) in a three-way PLS result plot based on variables. This option is used in connection with loading weights, variances, and variable plots. You cannot disable X1-, X2- and Y-variables simultaneously.

View - Source - Y-Variables

Shows or hides the Y-variables in a plot based on variables. This option is used in connection with loadings, variances, and variable plots. You cannot disable both X- and Y-variables.

View - Source - Explained Variance

Displays the explained variance for each PC, in a cumulative way, as a percentage of the initial variance. By definition, the explained variance for PC 0 is 0. The explained variance is expressed in percent and makes it easy to see how much of the total data variation is explained by the model.

View - Source - Residual Variance

Displays the residual variance for each PC. The residual variance plot is used to find the optimal number of components to use in the model. It is an expression of the modeling or prediction error.

View - Source - Y-residuals

Displays the raw Y-residuals of the current model. The residuals are the difference between the observed values and the values predicted by the model. The size of the residuals tells you about the amount of error in your model. A large residual shows that the sample is not well described by the model.

View - Source - Studentized Residuals

Displays the studentized residuals. Studentized residuals are scaled and corrected for leverage. The scaling makes the interpretation independent of the measurement units and the leverage correction increases the residuals for samples far from the model center.

View - Raw Data

When you select this option from a result Viewer, an Editor containing the raw data used to make the model you are looking at is displayed.

This Editor and the Viewer are linked so marked samples or variables in the Viewer are marked in the Editor, and vice versa. This is handy when you cannot find a sample or variable in the plot. Mark it in the Editor and you quickly see it in the plot.

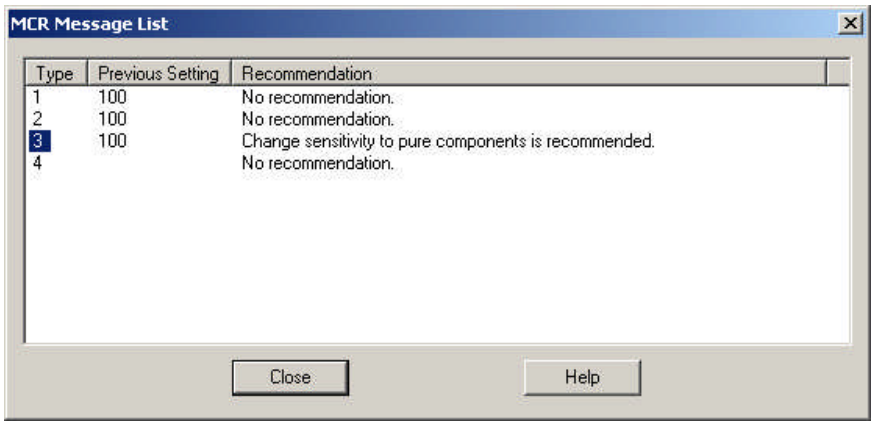
As the Sample Statistics and Variable Statistics tables, the Raw Data table behaves as a “slave”. It cannot be edited or plotted. If you want to freely manipulate the values in that table, you have to drag and drop its contents to an empty spot of the workplace.

View - MCR Message List...

This option is only available when viewing MCR results. It allows you to display the list of system-generated messages related to your MCR results.

The MCR message list appears in a separate window, as shown below.

The MCR Message List window



Check for any system recommendations:

- Recommendations of type 1-3 have to do with the value of field Sensitivity to Pure Components in the **Multivariate Curve Resolution (MCR)** dialog. Column Previous Setting displays the value you chose when specifying the MCR.
- Recommendations of type 4 are more general, e.g. “Data normalization is recommended”.

View - Outlier List…

This toggle selection lets you show or hide the outlier list.

This dialog displays the outlier warnings that The Unscrambler generated during analysis of the data tables or results you have plotted in the active Viewer. The tests that are performed are described in the Method References chapter, which is available as a .PDF file from CAMO’s web site www.camo.com/TheUnscrambler/Appendices .

The dialog consists of 7 columns. Below is a brief description of each column in the **Outlier List** dialog.

The columns in the Outlier List dialog

Columns	Description
PCs	The PC number for the current test is shown. The tests are calculated separately for each PC in the model.
Spls	The sample number is given for all positive tests that are related to samples.
Vars	The variable number for all positive tests that are related variables is given in this column.
OW#	Each test has its own warning number, so that you can see which warnings are generated from the same test.
Description	This column describes the test that was positive.
Limit	This is the limit that the test value is compared to. The limit can be changed in the Warning Limits dialog. You can access this dialog from each dialog where you make a model.
Value	This is the actual value that that was calculated for the test in question.

View - Toolbars…

This option lets you toggle the toolbars on and off, and is by default always enabled. The toolbars contain buttons giving you quick access to the most frequently used commands. You select which toolbars to display by selecting the appropriate check-boxes in the **Viewer Toolbars** dialog.

The toolbars can be moved to different locations. Click on the toolbar background with the left mouse button and drag it away. The toolbar is then “floating” and you can place it wherever you want on your desktop, also outside The Unscrambler.

View - Status Bar

This option is enabled by default, and toggles the status bar, which gives a lot of information, on and off. A check mark appears to the left of this command when the status bar is turned on.

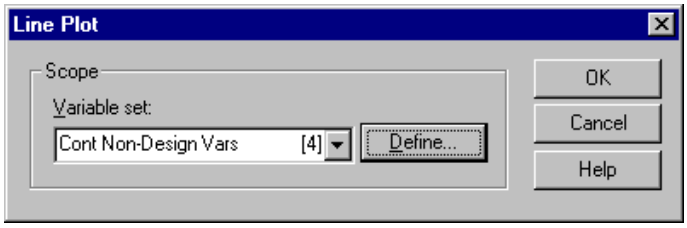
The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus and shows messages that describe the actions of toolbar buttons as you press them, before releasing them, while the right area indicates which user you are logged on as. The size of the data table and the value of the current cell is displayed when an Editor is active. It also tells whether you have read and/or write access to the data in the active window.

The Plot Menu

Plot - Line

The **Line** plot displays a data vector. When you are plotting from the Editor, you must mark the sample(s) or variable(s) you want to plot; one sample/variable gives a one-dimensional plot, specifying a range adds several line plots.

Dialog: Line Plot



You enter the **Line Plot** dialog where you must specify a Variable Set (if you have selected one or several samples), or a Sample Set (if you have selected one or several variables) from the drop-down list in the Scope field.

If necessary, press the Define button to define new sets in the **Set Editor**.

Use **Edit - Options** to change the layout of the plot.

Plot - 2D Scatter

The **2D Scatter** plot shows two data vectors plotted against each other. You enter the **2D/3D Scatter Plot** dialog where you can specify the scope of the plot.

Note:

When you are plotting from the Editor, you must mark the two samples or variables you want to plot, before using the **Plot** command.

In the **2D/3D Scatter Plot** dialog, specify a Variable Set (if you have selected two samples to plot), or a Sample Set (if you have selected two variables to plot) from the drop-down list in the Scope field.

If necessary, press the Define button to define new sets in the **Set Editor**.

Use **Edit - Options** to change the layout of the plot.

Plot - 3D Scatter

The **3D Scatter** plot shows three data vectors plotted against each other. You enter the **2D/3D Scatter Plot** dialog where you can specify the scope of the plot.

Note:

When you are plotting from the Editor, you must mark the two samples or variables you want to plot, before using the **Plot** command.

In the **2D/3D Scatter Plot** dialog, specify a Variable Set (if you have selected three samples to plot), or a Sample Set (if you have selected three variables to plot) from the drop-down list in the Scope field.

If necessary, press the Define button to define new sets in the **Set Editor**.

Use **Edit - Options** to change the layout of the plot.

Plot - Normal Probability

The **Normal Probability** plot shows the deviation from an assumed normal distribution of the data vector. It is not possible to plot more than one row or column at a time in this plot.

Select the sample or variable you want to plot and use **Plot - Normal Probability**. You enter the **Normal Probability Plot** dialog where you choose the scope of your plot.

Specify a Variable Set (if you have selected a sample to plot), or a Sample Set (if you have selected a variable to plot) from the drop-down list in the Scope field.

If necessary, press the Define button to define new sets in the **Set Editor**.

The data are plotted as a straight line through the point (0,50%), if they are normally distributed. Data points that are significantly different from the others deviate from the line and are placed in the upper right and lower left corner of the plot. You may add such a line manually by using **Edit - Insert Draw Item - Line**.

Use **Edit - Options** to change the layout of the plot.

Plot - Histogram

This plot displays the distribution of the data points in a data vector, as well as the normal distribution curve. A histogram gives useful information when you are exploring raw data. The height of each bar in the histogram shows the number of elements within the value limits of the bar. The normal distribution curve is useful when you want to see whether the distribution of your data is skewed. You may want to transform your variables if they are skewed in order to get a better model.

Select the sample or variable you want to plot and use **Plot - Histogram**. You enter the **Histogram Plot** dialog where you choose the scope of your plot.

Specify a Variable Set (if you have selected a sample to plot), or a Sample Set (if you have selected a variable to plot) from the drop-down list in the Scope field.

If necessary, press the Define button to define new sets in the **Set Editor**.

If you want another resolution of your histogram, you can change the number of bars to use in the plot using **Edit - Select Bars**. Use **Edit - Options** to change the layout of the plot.

Plot - Matrix

In this plot, a two-dimensional matrix is visualized. The plot is useful if you want to get an overview of your data before you start your analyses, as obvious errors in your data and outliers may be seen at once. You can also want to take a look at this plot before you decide whether to scale your data or not.

Select the sample(s) and/or variable(s) you want to plot in the Editor. If you select samples, you must specify which Variable Sets to plot in the **Matrix Plot** dialog, and vice versa. You can define new sets in the **Set Editor** by pressing the Define button. If you have selected the entire data table in the Editor, you can accept the default setup in the **Matrix Plot** dialog.

Four different layouts - landscape, bar, map, and contour - are available. Use **Edit - Options** to change the layout of the plot.

Plot - Matrix 3-D

Choose **Plot - Matrix 3-D** to display a matrix plot of one of the vectors in your 3-D data table.

With an OV^2 layout, you can produce a matrix plot of the Primary x Secondary variables for the plane represented by the selected sample.

With an O^2V layout, you can produce a matrix plot of the Primary x Secondary samples for the plane represented by the selected variable.

The **3-D Matrix Plot** dialog allows you to select which sample (resp. variable) to plot.

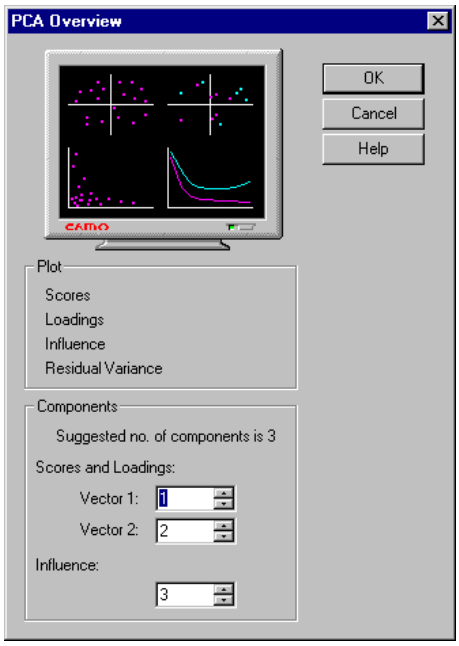
Four different layouts - landscape, bar, map, and contour - are available. Use **Edit - Options** to change the layout of the plot.

Plot - PCA Overview

The option **Plot - PCA Overview** gives you a quadruple plot of all the main results of a PCA, namely the scores, loadings, influence and total residual variance, as listed in the field Plot in the **PCA Overview** dialog, where you specify how to plot the overview.

In the Components field in the same dialog you specify which components to use for the scores and loadings and for the influence plot respectively.

Dialog: PCA Overview



Plot - Variances and RMSEP

There are three different ways to plot Variances and RMSEP against the number of components. You can plot:

1. X- or Y-variance;
2. X- and Y-variance (or X1- and X2-variance in the case of a three-way PLS model);
3. RMSE.

The last two options are only available if you have plotted regression results, the first one is also available for PCA results (with only X-variance available).

You specify what to plot in the dialog **Variances and RMSEP**, which contains one sheet for each of the possible plots listed above.

Variances and RMSEP Dialog: X- or Y-variance Sheet

This dialog sheet enables you to select either X-variances or Y-variances and display them as a single plot. Variance is plotted against component number. You can choose between calibration and validation samples, or both. Explained variance is selected by default; you can later change that by using **View - Source**.

In the field Variables, you select which variables you want to display in the plot. You can choose between variance for the X-variables or the Y-variables. To select All variables, click this button, and to enter an Editor where you can select variables, click Select. Tick the Total box to display the total variance at the same time.

You can decide whether you want the variance to be plotted for calibration or validation samples respectively, or both, by ticking the appropriate box(es) in the Samples field. Calibration variance measures the fit of the model to the calibration data. The validation variance is an estimate of the fit of the model to new data not present in the calibration, and is based on the validation. Plot both measures to obtain full information about model fit.

The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

Variances and RMSEP Dialog: X- or Y-variance Sheet (Three-Way PLS Results)

This dialog sheet enables you to select either Primary X (X1)-variances, Secondary X (X2)-variances or Y-variances and display them as a single plot. Variance is plotted against component number. You can choose between calibration and validation samples, or both. Explained variance is selected by default; you can later change that by using **View - Source**.

- In the field Variables, select which variables you want to display in the plot. You can choose between variance for the Primary X-variables, the Secondary X-variables or the Y-variables. To select All variables, click this button. Note that the Select button is disabled for three-way data.
  Tick the Total box to display the total variance at the same time.
- You can decide whether you want the variance to be plotted for calibration or validation samples respectively, or both, by ticking the appropriate box(es) in the Samples field. Calibration variance measures the fit of the model to the calibration data. The validation variance is an estimate of the fit of the model to new data not present in the calibration, and is based on the validation. Plot both measures to obtain full information about model fit.

The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

Variances and RMSEP Dialog: X- and Y-variance Sheet

This dialog sheet enables you to plot X- and Y-variances simultaneously, as a double plot.

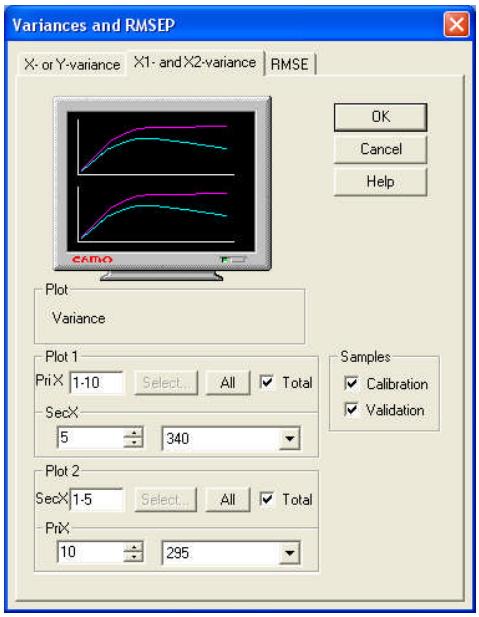
In the field Variables, you select which variables you want to display in the plot. You must select both X- and Y-variables. To select All variables, click this button, and to enter an Editor where you can select variables, click Select. Tick the Total box to display the total variance at the same time.

You can decide whether you want the variance to be plotted for calibration or validation samples respectively, or both, by ticking the appropriate box(es) in the Samples field. Calibration variance measures the fit of the model to the calibration data. The validation variance is an estimate of the fit of the model to new data not present in the calibration, and is based on the validation. Plot both measures to obtain full information about model fit. You can later change that choice by using **View - Source**.

Variances and RMSEP Dialog: X1- and X2-variance Sheet

This dialog sheet enables you to plot Primary X (X1)- and Secondary X (X2)-variances simultaneously, as a double plot. Variance is plotted against component number. You can choose between calibration and validation samples, or both. Explained variance is selected by default; you can later change that by using **View - Source**.

Dialog: Variances and RMSEP - X1- and X2-variance Sheet



- In the field Plot 1, select which Primary X-variables you want to display in the plot, for a fixed Secondary X-variable. To select All Primary X-variables, click the All button. Note that the Select button is disabled for three-way data. Tick the Total box to display the total variance at the same time. Choose as SecX the fixed Secondary X-variable that determines from which plane the selected Primary X-variable(s) is / are selected. You may either pick up the Secondary variable's number or its name.
- The field Plot 2 works in a similar way and allows you to select which Secondary X-variables you want to display in the plot, for a fixed Primary X-variable.
- You can decide whether you want the variance to be plotted for calibration or validation samples respectively, or both, by ticking the appropriate box(es) in the Samples field. Calibration variance measures the fit of the model to the calibration data. The validation variance is an estimate of the fit of the model to new data not present in the calibration, and is based on the validation. Plot both measures to obtain full information about model fit.

Variances and RMSEP Dialog: RMSE Sheet

This is a plot of the average prediction error, for either the calibration or the validation samples. In the plot you will find the Root Mean Square Error of Calibration (RMSEC) or Root Mean Square Error of Prediction (RMSEP) plotted against the number of components used in the model.

- If you select Calibration samples, the plot will display RMSEC.
- If you select Validation samples, the plot will display RMSEP.

In the field Variables, you select which Y-variables you want to plot. To select All variables, click this button, and to enter an Editor where you can select variables, click Select.

You can decide whether you want the variance to be plotted for calibration or validation samples respectively, or both, by ticking the appropriate box(es) in the Samples field. Calibration variance measures the fit of the model to the calibration data. The validation variance is an estimate of the fit of the model to new data not present in the calibration, and is based on the validation. Plot both measures to obtain full information about model fit. You can later change that choice by using **View - Source**.

The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

Plot - Sample Outliers

This quadruple plot is useful for visualizing sample outliers. Both validation and calibration samples are plotted in the Sample Variance and Score plots, while the influence plot contains only calibration samples.

In the **Sample Outliers** dialog, you must select the components for the Scores plot and Influence plot in the Components field. Start with the first few components or the component number where the prediction error starts to increase after a minimum.

Plot - Scores and Loadings

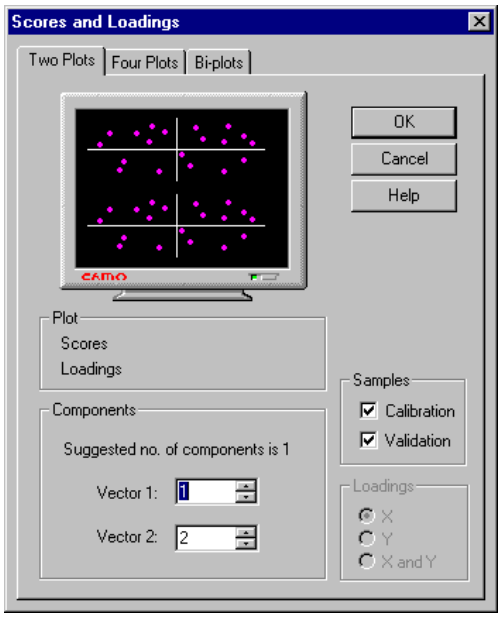
This is a quadruple plot of scores and loadings from a PCA or regression model. You will see the scores and loadings for two different sets of PCs. This plot is useful for interpreting the relationship between samples and variables in data.

There are three different ways to plot Scores and Loadings:

1. Two plots;
2. Four plots;
3. Bi-plots.

These are represented by different sheets in the **Scores and Loadings** dialog:

Dialog: Scores and Loadings



Scores and Loadings Dialog: Two Plots Sheet

This sheet lets you specify two plots, a Score plot in sub-view 2 and a Loadings plot in sub-view 3.

- Choose the PCs for which you want to look at the plots in the Components field.
- In the Samples field, select whether to plot Calibration and/or Validation samples.

- In the Loadings field, select whether to see X- or Y-loadings, or both.

Scores and Loadings Dialog: Four Plots Sheet

On this sheet you can specify four plots: two Score plots (plot 1 and plot 2) in sub-views 4 and 5 and two Loadings plots (plot 3 and plot 4) in sub-views 6 and 7.

- Specify four PCs in the Components field: the two axes common to plots 1 and 3 (first Scores plot and first Loadings plot) and the two axes common to plots 2 and 4.
- In the Samples field, select whether to plot Calibration and/or Validation samples.
- In the Loadings field, select whether to see X- or Y-loadings, or both.

Scores and Loadings Dialog: Bi-plots Sheet

Here, you can specify one plot which displays scores and X-loadings projected onto the same set of 2 PCs. You only need to specify which PCs to plot in the Components field.

Plot - Scores and Loading Weights

This is a quadruple plot of scores and loading weights from a three-way PLS model, along two selected PCs.

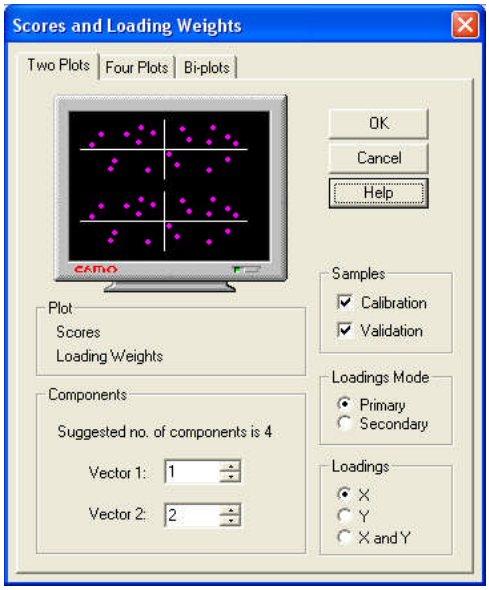
This plot is useful for interpreting the relationship between X-variables and Y-variables, while checking at the same time where the samples project. This may tell you about possible outliers or influential samples, and give you some hints as to which variables “explain” sample locations.

There are three different ways to plot Scores and Loading Weights:

1. Two plots;
2. Four plots;
3. Bi-plots.

These are represented by different sheets in the **Scores and Loading Weights** dialog:

Dialog: Scores and Loading Weights



Scores and Loading Weights Dialog: Two Plots Sheet

This sheet lets you specify two plots, a Score plot in sub-view 2 and a Loading Weights plot in sub-view 3.

- Choose the PCs for which you want to look at the plots in the Components field.
- In the Samples field, select whether to plot Calibration and/or Validation samples.
- In the Loadings Mode field, select whether to see Primary or Secondary X-variables.
- In the Loadings field, select whether to see X- or Y-loadings, or both.

Scores and Loading Weights Dialog: Four Plots Sheet

On this sheet you can specify four plots: two Score plots (plot 1 and plot 2) in sub-views 4 and 5 and two Loading Weights plots (plot 3 and plot 4) in sub-views 6 and 7.

- Specify four PCs in the Components field: the two axes common to plots 1 and 3 (first Scores plot and first Loading Weights plot) and the two axes common to plots 2 and 4.
- In the Samples field, select whether to plot Calibration and/or Validation samples.
- In the Loadings Mode field, select whether to see Primary or Secondary X-variables.
- In the Loadings field, select whether to see X- or Y-loadings, or both.

Scores and Loading Weights Dialog: Bi-plots Sheet

Here, you can specify one plot which displays scores and X-loading weights projected onto the same set of 2 PCs.

- Choose the PCs for which you want to look at the plots in the Components field.
- In the Loadings Mode field, select whether to see Primary or Secondary X-variables.

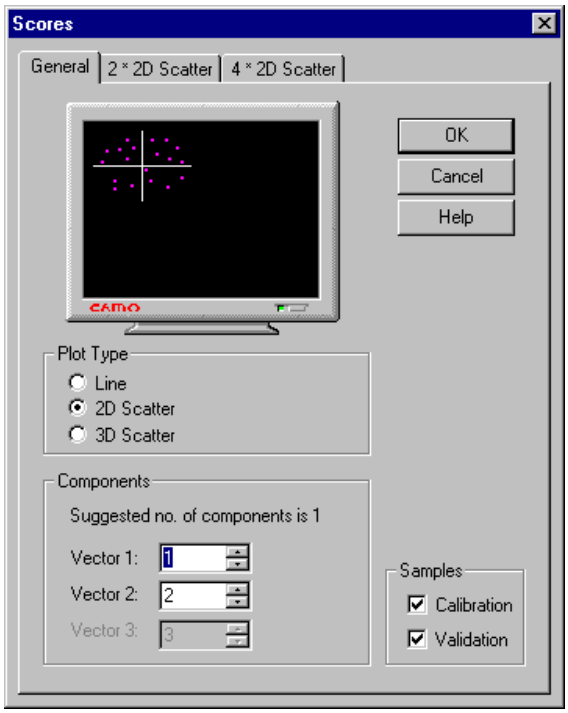
Plot - Scores

The score plot shows the similarities and differences among the samples, allowing you to investigate patterns and look for outliers.

The **Scores** dialog offers three different layouts for plotting, each available from its own sheet:

1. General (one plot window);
2. 2x2D Scatter (two windows);
3. 4x2D Scatter (four windows).

Dialog: Scores



Scores Dialog: General Sheet

On the General sheet in the **Scores** dialog, you specify one plot. You must decide whether you want a Line-, 2D Scatter- or 3D Scatter plot of the scores in the field Plot Type, and specify which components you want to see in the Components field. Use the default PCs 1 and 2 unless you have specific reasons for doing otherwise. Finally, make your choice in the Samples field. Calibration means that the scores from the calibration samples, i.e. the samples used to construct the model, will be plotted. If you have used a test set validation in the computations, you can also choose Validation which will give you the scores for the validation samples.

The preview screen on the sheet lets you switch between displaying the plot in the upper left corner of the screen and on the entire screen. Double click in the preview screen to switch between the options.

Scores Dialog: 2 x 2D Scatter Sheet

This sheet lets you specify two 2D Scatter plots, which are displayed horizontally. The number of components must be selected for each sub-window.

Specify which components you want to see in the Components field. Then, make your choice in the Samples field. Calibration means that the scores from the calibration samples, i.e. the samples used to construct the model, will be plotted. If you have used a test set validation in the computations, you can also choose Validation which will give you the scores for the validation samples.

Scores Dialog: 4 x 2D Scatter Sheet

This sheet lets you specify four 2D Scatter plots. The number of components must be selected for each sub-window.

Specify which components you want to see in the Components field. Then, make your choice in the Samples field. Calibration means that the scores from the calibration samples, i.e. the samples used to

construct the model, will be plotted. If you have used a test set validation in the computations, you can also choose Validation which will give you the scores for the validation samples.

Plot - Loadings

The loading plot shows which variables are important and which variables correlate.

The command **Plot - Loadings** launches the **Loadings** dialog where you can choose between three different sub-view layouts for plotting, and select various options (type of plot, variables, PCs).

Loadings Dialog and Loading Weights Dialog

The **Loadings** and **Loading Weights** dialogs offer three different layouts for plotting, each available from its own sheet:

1. General (one plot window for PCA, PCR and PLS – two windows for three-way PLS);
2. 2x2D Scatter (two windows);
3. 4x2D Scatter (four windows).

Loadings / Loading Weights Dialog: General Sheet

On the General sheet (which is active by default), you specify either:

- ***one plot*** if you are viewing ***PCA, PCR or PLS*** results. The plot will be displayed either in the currently active sub-view, or in sub-view #1.
- ***two plots*** if you are viewing ***three-way PLS*** results. The plots will show results along the same couple of PCs for resp. Primary and Secondary variables in the upper and lower sub-view. Note that if you choose only Y-variables (see the options below), only one plot will be produced, in the upper sub-view.

You must decide whether you want a Line-, 2D Scatter- or 3D Scatter plot in the field Plot Type, and specify along which components you want the results in the Components field. Use the default values 1 and 2 unless you have specific reasons for doing otherwise.

Finally, make your choice between plotting either X-, Y- or both X- and Y-variables in the Variables field.

When plotting PCA, PCR or PLS results, the ***preview screen*** on the sheet lets you switch between displaying the plot in one of the 4 corners of the screen and on the entire screen. Double click in the preview screen to switch between the options; this way you decide whether the plot will appear in a small or large sub-view.

Specific to Loading Weights:

For ***Y-variables*** in a PLS model, ***Loadings*** will be plotted since Loading Weights exist only for X-variables. Choosing "X- and Y-variables" will produce a plot of X-Loading Weights and Y-Loadings.

For three-way PLS however, since there are no loadings, Loading Weights are plotted for both X- and Y-variables.

Loadings / Loading Weights Dialog: 2 x 2D Scatter Sheet

This sheet lets you specify two 2D Scatter plots, which are displayed in sub-views #2 and 3.

The number of components must be selected for each sub-window.

Specify which components you want to see in the Components field.

Finally, make your choice between plotting X-, Y- or X- and Y-variables in the Variables field.

Specific to Loading Weights:

For ***Y-variables***, ***Loadings*** will be plotted since Loading Weights exist only for X-variables. Choosing "X- and Y-variables" will produce a plot of X-Loading Weights and Y-Loadings.

Loadings / Loading Weights Dialog: 2 x 2D Scatter Sheet (Three-Way PLS Results)

This sheet lets you specify two 2D Scatter plots, which are displayed in sub-views #2 and 3.

The number of components must be selected for each sub-window.

- In the Components field, specify along which components you want the results to be plotted.
- In the X-variable Mode field, choose between Primary and Secondary X-variables.
- Finally, make your choice between plotting X-, Y- or X- and Y-variables in the Variables field.

Loadings / Loading Weights Dialog: 4 x 2D Scatter Sheet

This sheet lets you specify four 2D Scatter plots.

The number of components must be selected for each sub-window.

Specify which components you want to see in the Components field.

Finally, make your choice between plotting X-, Y- or X- and Y-variables in the Variables field.

Specific to Loading Weights:

For ***Y-variables***, ***Loadings*** will be plotted since Loading Weights exist only for X-variables. Choosing "X- and Y-variables" will produce a plot of X-Loading Weights and Y-Loadings.

Loadings / Loading Weights Dialog: 4 x 2D Scatter Sheet (Three-Way PLS Results)

This sheet lets you specify four 2D Scatter plots, which are displayed in sub-views #4 to 7.

The number of components must be selected for each sub-window.

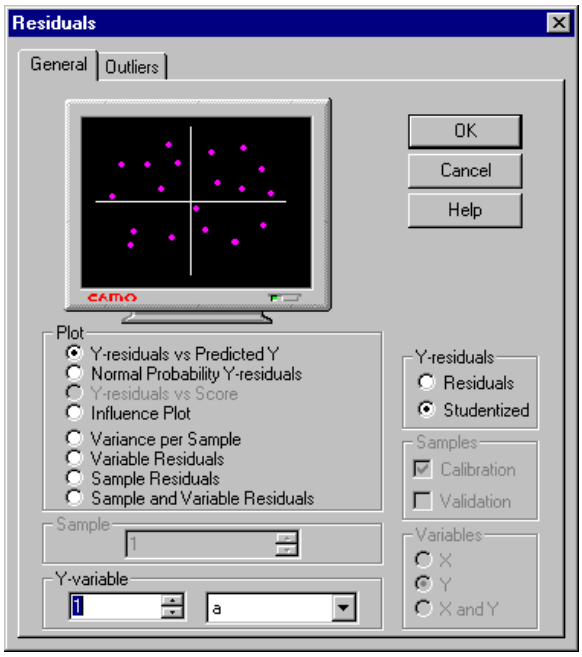
- In the Components field, specify along which components you want the results to be plotted.
- In the X-variable Mode field, choose between Primary and Secondary X-variables.
- Finally, make your choice between plotting X-, Y- or X- and Y-variables in the Variables field.

Plot - Residuals

Residuals are the deviations between the observed data values and the model approximation of those values. An object (sample or variable) with large residuals is not well described by the model. Residuals should be small and have no pattern. The plots of Y-residuals are only available for Regression, Analysis of Effects and Response Surface results.

The **Residuals** dialog consists of up to three sheets: General, Outliers, and Patterns. The Patterns sheet is available for Regression results only. The Outliers sheet is not available for PCA. In the case of a Multivariate Curve Resolution (MCR) the two sheets are: MCR Fitting and PCA Fitting.

Dialog: Residuals, Analysis of Effects



Residuals Dialog: General Sheet

In the Plot field on the General sheet you must choose which type of plot you want to make by selecting the appropriate radio button. You have 8 choices, as described below.

Plots in the Residuals dialog; General sheet

Plot type	Description
Y-residuals vs. Predicted	Useful to detect outliers and/or lack of model fit, and systematic errors.
Normal Probability Y-residuals	A normal probability plot of the Y-residuals which is useful to detect lack of model fit.
Y-residuals vs. Score	A plot of Y-residuals vs. component scores which is another way to detect lack of fit in the model.
Influence Plot	Squared residuals are plotted against leverage. When a regression is performed you can use it both for X and Y-variables. The plot is useful for outlier detection.
Variance per Sample	A plot of the average squared residual for each calibration sample taken over variables. It is useful to detect outliers.
Variable Residuals	A plot of residuals versus sample number for selected variables, used to detect outliers and lack of model fit.
Sample Residuals	A plot of residuals versus variable number for selected samples, useful for detecting outliers and models with bad fits.
Sample and Variable Residuals	A matrix plot of residuals for samples and variables and another way to detect outliers or lack of fit.

Choose which samples and variables you want to plot in the Sample and Y-Variable fields respectively. In addition, for PCA, PCR and PLS results, all the plots require that you select a number of components in the Components field. You will then see the residuals for a model consisting of this number of components.

Choose between raw residuals or studentized residuals in the Y-residuals field, and between calibration or validation samples in the Samples field. Finally, select X-variables, Y-variables or both in the Variables field. The Y-variable option is not available for PCA results.

Residuals Dialog: General Sheet (Three-Way PLS Results)

In the Plot field on the General sheet you must choose which type of residual plot you want to display by selecting the appropriate radio button. You have 7 choices, as described hereafter.

Plots in the Residuals dialog; General sheet (Three-Way PLS Results)

Plot type	Description
Y-residuals vs. Predicted	Useful to detect outliers and/or lack of model fit, and systematic errors.
Normal Probability Y-residuals	A normal probability plot of the Y-residuals which is useful to detect lack of model fit.
Y-residuals vs. Score	A plot of Y-residuals vs. component scores which is another way to detect lack of fit in the model.
Influence Plot	Squared residuals are plotted against leverage. When a regression is performed you can use it both for X and Y-variables. The plot is useful for outlier detection.
Variance per Sample	A plot of the average squared residual for each calibration sample taken over variables. It is useful to detect outliers.
Variable Residuals	A plot of residuals versus sample number for selected variables, used to detect outliers and lack of model fit.
Sample Residuals	A plot of residuals versus variable number for selected samples, useful for detecting outliers and models with bad fits.

The options available beside and below the Plot field may vary depending on the type of plot you have chosen. All possible options are described hereafter.

- In the Y-residuals field, choose between raw residuals or studentized residuals.
- In the Sample field, select for which sample you want to display Sample residuals.
- In the Primary X-Variable, Secondary X-Variable and Y-Variable fields, choose the appropriate variable(s).
- In the Samples field to the right (available for Y-residuals vs Predicted Y and Variance per Sample, select Calibration, Validation or both types of Samples.
- In the X-Variable Mode field to the right (available for Variable Residuals with additional choice "X"), select Primary, Secondary or both types of X-variables. Selecting both will produce a line plot showing all samples for the selected (X1,X2). Selecting only one mode will produce a matrix plot combining all samples with all variables from the other mode.
- In the Variables field to the bottom right, choose either X-variables, Y-variables or both.
- In the Components field at the bottom, choose the number of components for which you want the results displayed. The All button allows you to plot results for all PCs simultaneously – but the plot may be quite messy!

Residuals Dialog: Outliers Sheet

From the Outliers sheet you can produce a double plot showing an Influence Plot and a Y-residuals vs Predicted Y plot. It is tailor-made for easy visualization of outliers and their influence on the calibration model.

Choose which Y-variable you want to investigate from the list in the Y-variable field and, in the Components field, the components you want to examine for outliers. You must also decide whether to look at the X-, Y-, or both variables in the Variables field.

Residuals Dialog: Patterns Sheet

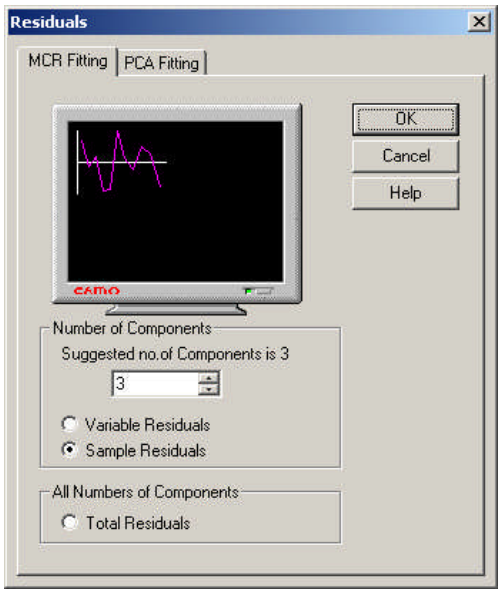
On the Patterns sheet you can produce a double plot showing Normal Probability of Y-residuals and Y-residuals vs. Score. This is an excellent way to visualize possible clear patterns (for instance curvature or systematic errors) in the Y-residuals when a regression analysis is performed. Such structures can indicate a lack of model fit.

Choose which Y-variable you want to investigate from the list in the Y-variable field and, in the Components field, the components you want to examine for outliers. You must also decide whether to take into account the calibration and/or validation samples in the Samples field.

Residuals Dialog: MCR Fitting Sheet

From the MCR Fitting sheet (available only for MCR results) you can produce a line plot showing the Variable, Sample or Total residuals which summarize the quality of the MCR fitting.

Dialog: Residuals, MCR



- In the Number of Components field, choose the number of components for which you want to display Variable or Sample residuals.
  A radio button allows you to toggle between Variable Residuals and Sample Residuals.
- Alternatively, field All Numbers of Components allows you to display Total Residuals for each model component. The abscissa of the plot will have as many values as there are components in the model.

Residuals Dialog: PCA Fitting Sheet

From the PCA Fitting sheet (available only for MCR results) you can produce a line plot showing the Variable, Sample or Total residuals which summarize the quality of a PCA fitting on your MCR data. Use these plots to compare the quality of your MCR fitting to that of a PCA fitting.

- In the Number of Components field, choose the number of components for which you want to display Variable or Sample residuals.
  A radio button allows you to toggle between Variable Residuals and Sample Residuals.
- Alternatively, field All Numbers of Components allows you to display Total Residuals for each model component. The abscissa of the plot will have as many values as there are components in the model.

Plot - Leverage

Leverages are useful for the detection of samples which are far from the center within the space described by the model. If a sample has a very large leverage, it may be different from the rest and can be considered to be an outlier. Large leverage indicates a high influence on the model.

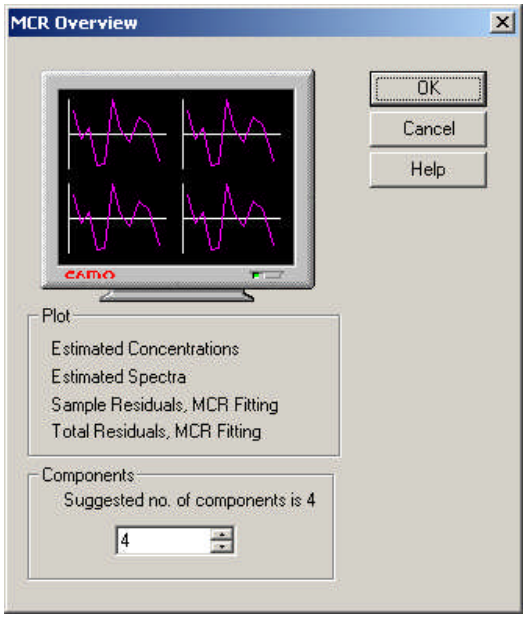
In the **Leverage** dialog, choose a Line or a Matrix plot in the Plot field. The Line plot presents the leverages for each sample, while the Matrix plot shows the leverages for different samples and components.

If you select a Line plot, you must also choose the number of components in the Components field and, if the Samples field is enabled, whether you want to see the calibration and/or validation samples.

Plot - MCR Overview

Accessed with the command **Plot - MCR Overview**, this command produces a quadruple plot of the main results of a Multivariate Curve Resolution (MCR). These are: Estimated Concentrations, Estimated Spectra, Sample Residuals (MCR Fitting) and Total Residuals (MCR Fitting) as shown in the Plot field of the **MCR Overview** dialog.

Dialog: MCR Overview



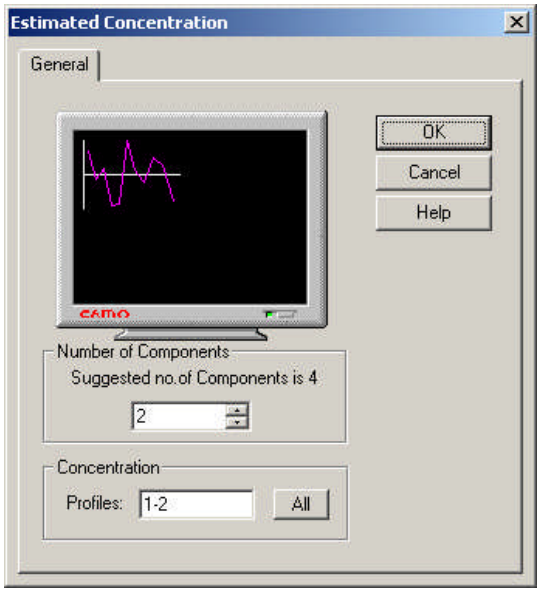
In the Components field you may tune up or down the number of components for which the results will be plotted.

Plot - Estimated Concentrations

Accessed with the command **Plot - Estimated Concentrations**, this command produces a line plot of the Estimated Concentrations in your Multivariate Curve Resolution (MCR) results.

The **Estimated Concentrations** dialog contains only one sheet called “General”.

Dialog: Estimated Concentrations



In the Number of Components field you may tune up or down the number of components for which the Estimated Concentrations will be plotted.

In the Concentration field you choose which profiles to display. These are the Estimated Concentration profiles of each constituent, plotted across all the samples included in the analysis. Use the All button to display the profiles of all the estimated constituents.

Plot - Estimated Spectra

Accessed with the command **Plot - Estimated Spectra**, this command produces a line plot of the Estimated Spectra in your Multivariate Curve Resolution (MCR) results.

The **Estimated Spectra** dialog contains only one sheet called “General”.

In the Number of Components field you may tune up or down the number of components for which the Estimated Spectra will be plotted.

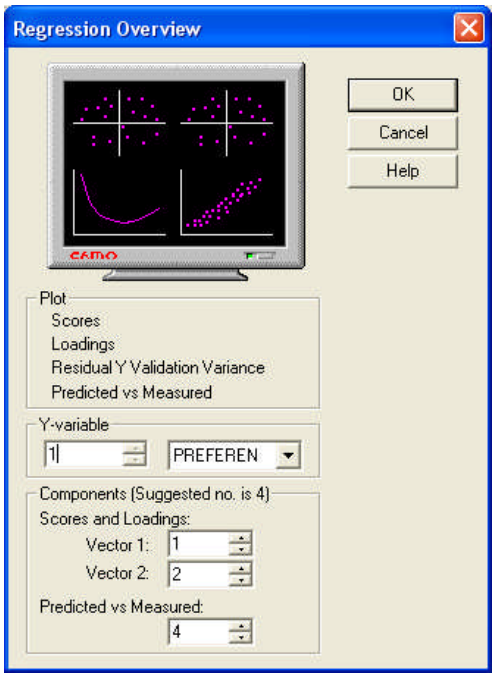
In the Spectra field you choose which profiles to display. These are the Estimated Spectra of each pure constituent, plotted across all the variables included in the analysis. Use the All button to display the profiles of all the estimated constituents.

Plot - Regression Overview

Accessed with the command **Plot - Regression Overview**, this is a quadruple plot of some of the main results of a PCR or PLS regression, namely the scores and loadings, X- and Y-loadings, residual Y-variance

(validation) and predicted versus measured Y-value as shown in the Plot field in the **Regression Overview** dialog.

Dialog: Regression Overview



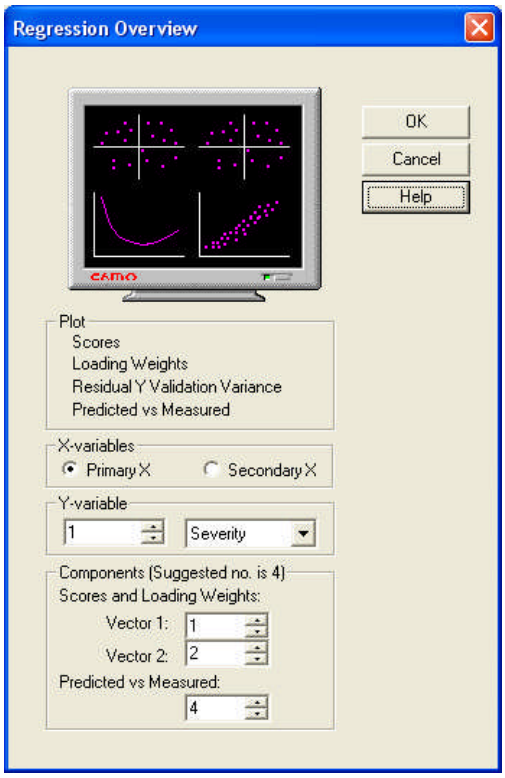
In the field Y-variable you choose which Y-variable to study, and in the Components field you choose the PCs to be used as axes for Scores and Loadings, and the number of components for Predicted versus Measured (the latter should be the optimal number of PCs).

If the X-variable Set used to generate the regression results is of type Spectra, the **Regression Overview** dialog has a slightly different composition: the 2D scatter plot of X and Y-loadings is replaced with a line plot of the regression coefficients.

Regression Overview Dialog: Three-Way PLS Results

Accessed with the command **Plot - Regression Overview** when viewing three-way PLS results, this dialog allows you to produce a quadruple plot of the main results, namely scores, X- and Y-loading weights, residual Y-variance (validation) and predicted versus measured Y-value, as shown in the Plot field in the **Regression Overview** dialog.

Dialog: Regression Overview for Three-Way PLS results



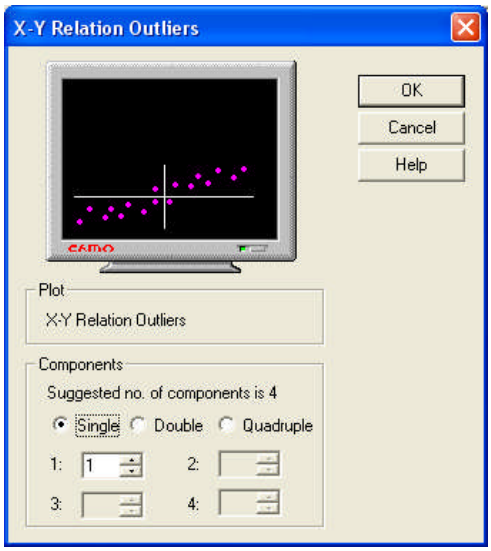
- In the X-variables field, choose whether to display Primary or Secondary X-variables.
- In the Y-variable field, choose which Y-variable to study.
- In the Components field, choose the PCs to be used as axes for Scores and Loading Weights, and the number of components for Predicted versus Measured. It is recommended to use the optimal number of PCs for plotting Predicted vs Measured.

Plot - X-Y Relation Outliers

This is a plot of t-scores vs u-scores which can be used to detect outliers in PLS. The samples should lie as close to each other as possible along a straight line through most of the samples. Samples that stick out from this line are possible outliers.

The plot is specified in the dialog **X-Y Relation Outliers**, where you have to choose between single, double or quadruple plots (giving 1, 2 or 4 components) in the Components field. In each case, you also need to select the correct number of components.

Dialog: X-Y Relation Outliers

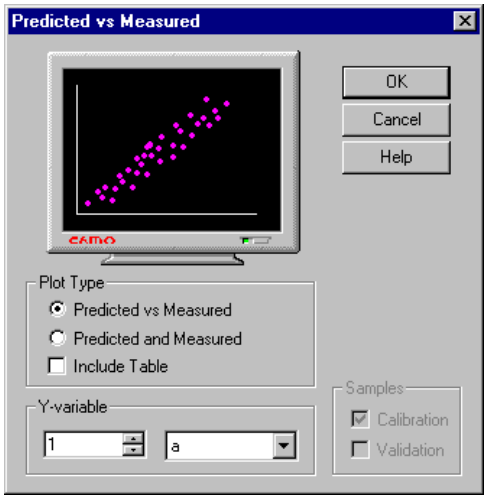


Change the size of the plot by double-clicking in the preview screen in the dialog.

Plot - Predicted vs Measured

In this plot, the measured Y-values and the predicted Y-values are plotted. This is useful to check the quality of the regression model fitted to the data. Predicted values should be as similar as possible to the measured values.

Dialog: Predicted vs Measured



In the **Predicted vs Measured** dialog, choose which plot you want to make in the Plot Type field. You have two options:

- Predicted vs Measured, which plots the predicted Y-values versus the measured Y-values for all samples;

- Predicted and Measured, which is a plot of Y-values, with one curve showing the measured values and another showing the predicted values.

In addition, you must tick the box Include Table if you want to include a table plot of the predicted and measured values. In that case, the plot will be displayed in sub-view 2 and the table plot in sub-view 3.

Then, select which Y-variable you want to see the results from in the Y-variable field and the number of components in the Components field. Finally, select calibration and/or validation samples in the Samples field.

If you have not included the table plot, you can change the size of the plot by double-clicking in the preview screen in the dialog.

Plot - Loading Weights

The loading weights plot is available for PLS1, PLS2 and three-way PLS results only. It shows which variables are important for the prediction of Y. For PLS results, X-loading weights should usually be plotted together with Y-loadings.

The command **Plot - Loading Weights** launches the **Loading Weights** dialog (see p.185) where you can choose between three different sub-view layouts for plotting, and select various options (type of plot, variables, PCs).

Plot - Important Variables

This double plot combines regression coefficients (Bw) and loadings (loading weights if it is a PLS1, PLS2 or three-way PLS model). The plot can be useful for detecting the most important variables.

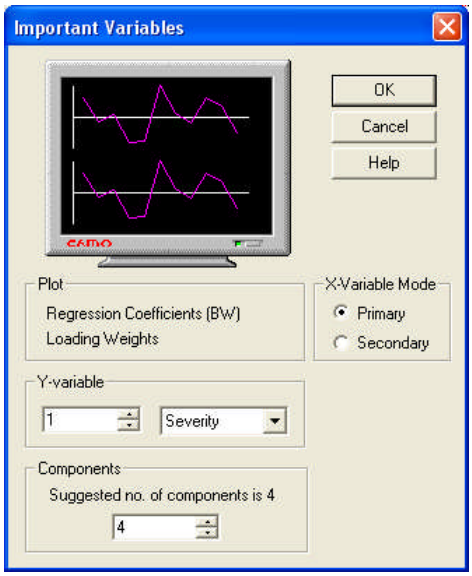
Plot Important Variables - PCR, PLS1 and PLS2 Results

In the **Important Variables** dialog, select the Y-variable for which you want to to display the regression coefficients in the Y-variable field. You must also select the number of components for the computation of the coefficients in the Components field. The regression coefficients are summarized for all components up to and including the chosen number. For the loadings, all components up to and including the chosen number are plotted in one sub-view.

Plot Important Variables - Three-Way PLS Results

In the **Important Variables** dialog you may configure your double plot of Regression Coefficients and Loading Weights.

Dialog: Important Variables (Three-Way PLS Results)



- In the X-variable mode field, choose between Primary and Secondary variables. This will only affect the plot of Loading Weights; the Regression Coefficients will be plotted as a matrix showing X1- and X2-variables together.
- In the Y-variable field, select the Y-variable for which you want to display the regression coefficients.
- In the Components field, select the number of components taken into account for the computation of the regression coefficients. The regression coefficients are summarized for all components up to and including the chosen number. For the loading weights, all components up to and including the chosen number are displayed as a line plot in the lower sub-view.

Plot - Regression Coefficients

You can plot the regression coefficients from a multiple linear regression (MLR) analysis, or from a PCR or PLS regression analysis. This is done in the **Regression Coefficients** dialog, where you have to select the Plot Type (line or matrix), the Y-variable and - for PCR, PLS and three-way PLS - the number of Components you want to include in your analysis.

Plot Regression Coefficients - MLR and Response Surface

Plotting the regression coefficients from a multiple linear regression analysis can be useful for interpreting the relationship between Y and all the X-variables.

The regression coefficients are used to compute new Y-values according to the equation (for a linear model; in addition the model may have interactions and / or squares):

$$y = b_0 + b_1x_1 + b_2x_2 + \ldots + b_Kx_K + f$$

For MLR, you can include the information listed below in the plot:

Information which can be included in an MLR regression coefficients plot

Options	Description
t-values	The t-values for the hypothesis that a regression coefficient is equal to 0 are used.
p-values	The p-values corresponding to the observed t-values are plotted.
Standard error	The standard errors of the regression coefficients are plotted.

The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

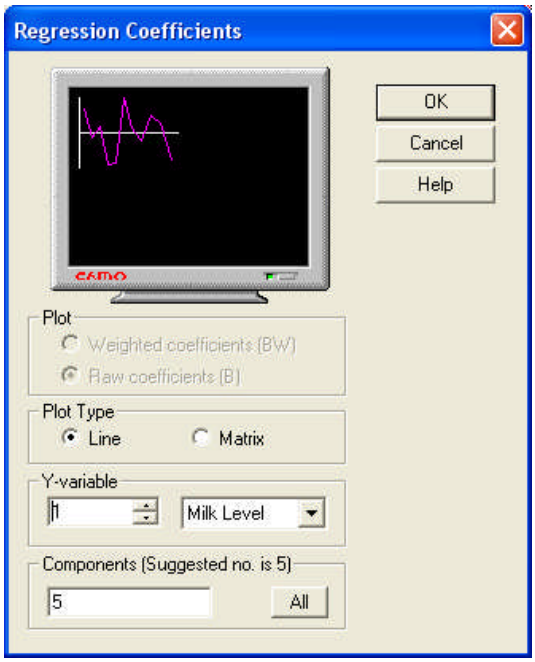
Plot Regression Coefficients - PCR and PLS

The regression coefficients (Bw = scaled or B = unscaled) from a PCR or PLS regression analysis are plotted.

The scaled regression coefficients take into account the weighting options you have chosen when specifying your regression analysis. They can help you identify the important X-variables in relationship with a given Y-variable.

In the **Regression Coefficients** dialog, you have to specify the number of Components in addition to the other options.

Dialog: Regression coefficients, PLS



The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

Note: Once the plot of regression coefficients is displayed, you may use options **View - Uncertainty Test - Uncertainty Limits** and **Edit - Mark - Significant X-Variables Only** to study the significance of your X-variables (available only if you have chosen the "Uncertainty Test" option in the Regression dialog upon specifying your regression model).

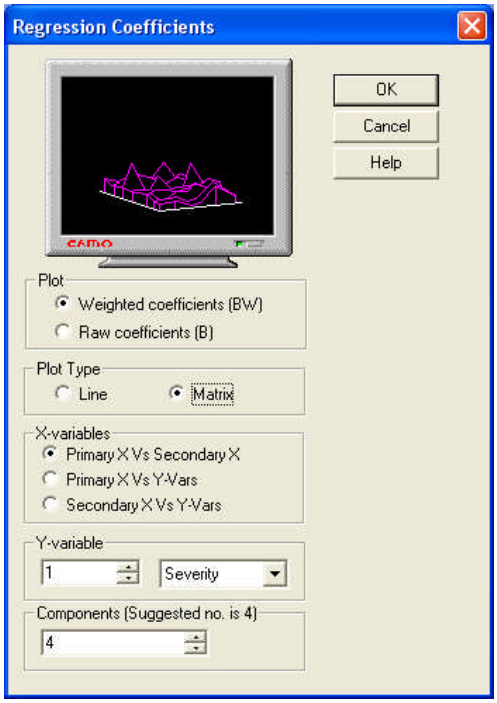
Plot Regression Coefficients - Three-Way PLS

The regression coefficients (Bw = weighted = scaled or B = raw = unscaled) from a three-way PLS model are plotted.

The scaled regression coefficients take into account the weighting options you have chosen when specifying your three-way analysis. They can help you identify the important X-variables in relationship with a given Y-variable. If you chose not to weight the X-variables, the Bw coefficients are identical to the Bs.

The **Regression Coefficients** dialog allows you to specify various options in addition to the type of coefficients.

Dialog: Regression coefficients, PLS



- In the Plot Type field, choose between a Line plot and a Matrix plot. This will affect the options below.
- In the X-variables field, select the variables to plot.
  If your plot type is a Line plot, choose between Primary and Secondary variables.
  If your plot type is a Matrix plot, you may choose to combine Primary and Secondary X-variables (for a fixed Y), or to vary Y (if your model includes several Y-variables) and combine it with either Primary or Secondary Xs.
- In the Y-variable field, select the Y-variable for which you want to display the regression coefficients.
- In the Primary X-variable field (available for a Matrix plot of Secondary X- Vs Y-vars), select the X1-plane for which you want to display the regression coefficients.
- In the Secondary X-variable field (available for a Matrix plot of Primary X- Vs Y-vars), select the X2-plane for which you want to display the regression coefficients.
- In the Components field, select the number of components taken into account for the computation of the regression coefficients. The regression coefficients are summarized for all components up to and including the chosen number. For the loading weights, all components up to and including the chosen number are displayed as a line plot in the lower sub-view.

The dialog displays a ***preview screen***. Double-click on this to change the size of the plot.

Plot - Regression and Prediction

This option produces a double plot of both regression coefficients (BW for PCR and PLS, B for MLR) and predicted values. Regression coefficients are used to interpret the relationship between the Y- and X-variables. The plot of the predicted Y versus the measured Y indicates the predictive quality of the regression function. For MLR, you can include the t-values and/or p-values for the regression coefficient. In such cases, the plot becomes a quadruple plot.

In the **Regression and Prediction** dialog, specify whether you wish to plot t- or p-values in the Plot field. Then, specify the Y-variable for which you want to look at the coefficients and predicted values in the Y-variable field and decide whether to include Calibration and/or Validation in the analysis (Samples field).

Plot - Response Surface

This plot visualizes the relationship between one Y-variable and a selection of two X-variables(*) as a contour or a landscape plot. You see how the response (Y) varies as a function of the selected X-variables, all other variables are kept at constant levels, which are the mean levels by default.

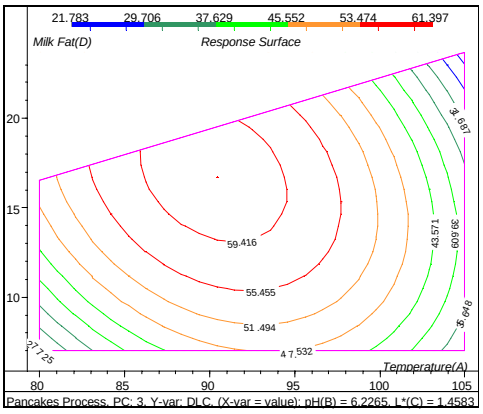
(*) Three X-variables in the case of mixtures.

The Contour Plot shows the contours or level curves of the surface. The optimum value will be indicated if it is within the experimental region.

The Landscape Plot shows the surface in a three-dimensional plot with the X-variables in the horizontal plane and the fitted response in the vertical direction.

All response surfaces plotted in the **Contour plot** layout display values for the Y-variable along the contour lines. These values are expressed in the unit of the Y-variable. They come in addition to the use of several colors; they are of major interest, in particular if you wish to print out a contour plot on a black and white printer.

Contour Plot of a D-Optimal Design. Values are displayed along the contour lines



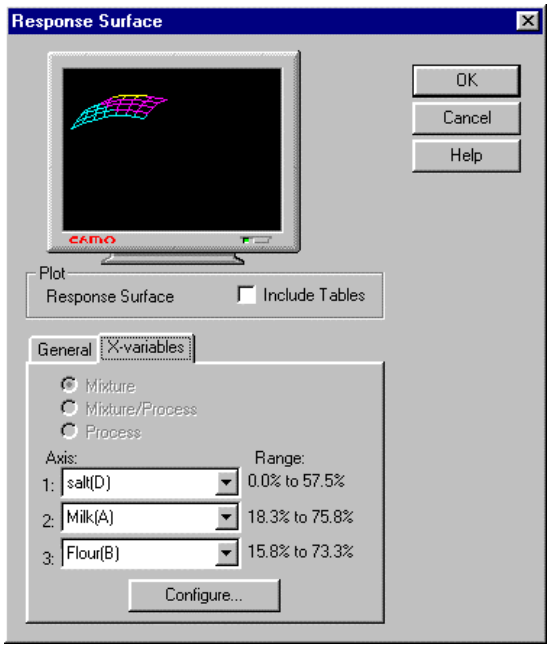
Note: All contour plots display values along the contour lines, regardless of the type of data plotted.

Plot Response Surface: Response Surface Dialog

In the Plot field in the **Response Surface** dialog, you can choose whether or not to include a table which shows the measured and predicted values of the Y-variable plus the standard error of the prediction for each sample. This will automatically place the plot itself in sub-view 2 and the table in sub-view 3.

If you have not included the table plot, you can change the size of the plot by double-clicking in the preview screen in the dialog.

Dialog: Response Surface



In addition, the **Response Surface** dialog contains two sheets:

1. General;
2. X-variables.

Response Surface Dialog : General Sheet

In the General sheet, three fields must be configured: Layout, Y-variable and Components.

In the Layout field you make your choice between the two plot types.

Then, define the Y-variable you want to investigate in the Y-variable field.

Finally, set the number of Components in this field.

Response Surface Dialog : X-variables Sheet

The X-variables sheet lets you select the type of plot you need and choose relevant X-variables.

Three types of plot are available, corresponding to the following situations:

1. Mixture
2. Mixture / Process
3. Process

Mixture

Select this plot type if you want to build a response surface with three mixture variables varying. The other mixture variables and all process variables are fixed. This plot is available only if your analysis included mixture variables.

Note: This plot has a triangular shape, and displays the mixture variable names and ranges of variation.

Mixture / Process

Select this plot type if you want to build a response surface with one process variable and one mixture variable varying. The other mixture variables are varied so that all the coordinates of the surface lie along the selected mixture variable axis. All process variables except the varied one are fixed. This plot is available only if your analysis included mixture variables and at least one process variable.

Process

Select this plot if you want to build a response surface with two independent process variables (i.e. non-mixture variables) varying. All the other process variables and all mixture variables are fixed. This plot is available only if your analysis included two or more process variables.

Note: The Process and Mixture type plots are able to handle multi-linear constraints. A border is drawn around the actual experimental region and only the points belonging to this region are drawn.

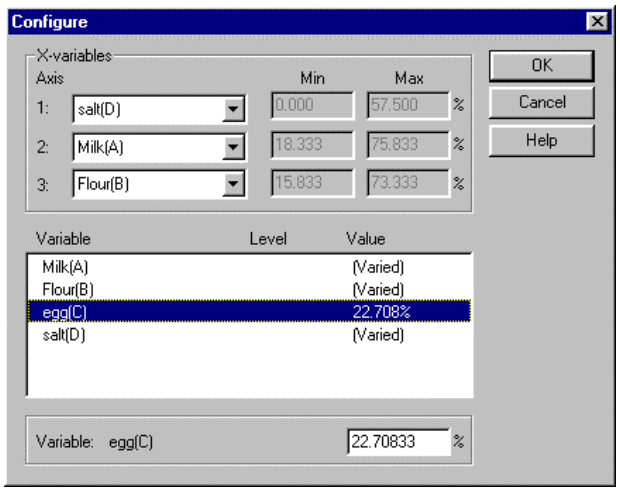
Configure Ranges of Variation

Once you have chosen the type of plot to use, select which X-variables you want to vary with the combo boxes. Use the Configure to invoke the **Configure** dialog, where you can set up which X-variables vary along the axes and which constant values the others should take.

Plot Response Surface: Configure Dialog

In the **Configure** dialog you can change the ranges of variation (for the varying variables) and the fixed values (for the non-varying variables).

Dialog: Configure



Choose which variables you want on axis 1 and axis 2 (and axis 3 for a mixture plot) of the response surface plot from the drop-down lists in the X-variables field.

The Min and Max boxes enable you to select the ranges of variation for the varied X-variables; these boxes are disabled when making a response surface plot from designed data.

The other X-variables are by default set to their mean value. You can change this by selecting the variable from the list in the Variable field and using the spin buttons on level and value. If a category variable is chosen, the spin button changes to a list of the available levels.

Plot - Response Surface Overview

This is a quadruple plot of some of the main results of a response surface analysis, namely the ANOVA table for the effects, the normal probability plot of the residuals, a contour plot, and a landscape plot of the surface itself. This overview is displayed for one Y-variable. For the contour and landscape plots, the most significant X-variables (the ones with the largest absolute B coefficients) are used if the number of X-variables is larger than two. Axes not shown are set to their average values.

You only have to make one choice in the **Response Surface Overview** dialog: Choose which Y-variable to study in the Y-variable field.

Plot - Analysis of Variance

This plot displays the ANOVA table which tells you about the significant effects in the model. If you are displaying results from an **Analysis of Effects** with variables having more than two levels, the same plot dialog also enables you to plot multiple comparisons. This is a comparison of the average responses for the different levels of a design variable which is useful in determining which levels of a variable are responsible for a possible significant effect.

The ANOVA table shows degrees of freedom, sums of squares, mean squares, f-values, and p-values for all variables, as well as interactions if they are used in the model. The Multiple Correlation and the r-square are also presented. If the results come from a response surface, a model check and a lack of fit test will be shown below the ANOVA table for the effects. In the latter case, intercept terms and max/min/saddle points are also given.

The plot can be generated from a response surface analysis, an analysis of effects or a regression analysis using MLR. The **Analysis of Variance** dialog will be slightly different depending on the number of levels studied for the (design) variables.

Analysis of Variance Dialog: General Case

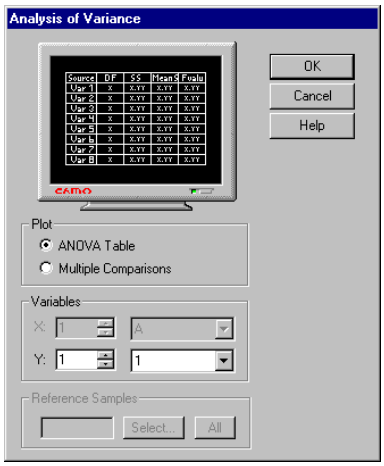
In the Variables field of the **Analysis of Variance** dialog, simply select the response variable (Y-variable) of interest.

Double-click on the plot preview in the dialog if you want the plot to be displayed on a larger (resp. smaller) sub-view.

Analysis of Variance Dialog: Multiple-Level Analysis of Effects

In designs which contain variables with more than two levels, i.e. Full Factorial designs, you must select whether you want to plot an ANOVA table or Multiple Comparisons with the radio buttons in the Plot field in the **Analysis of Variance** dialog, as seen in the figure below. Then, select the response variable (Y-variable), and, for Multiple Comparisons, the X-variable, in the Variables field, and decide whether you want the reference samples indicated in the multiple comparisons plot.

Dialog: Analysis of Variance, multilevel AoE



Plot - Effects

This option lets you plot an overview table of the effects of all design variables on all the responses.

There are three sheets in the **Effects** dialog: Overview, Response Details and Effect Details.

Effects Dialog: Overview Sheet

On this sheet you can specify a table plot which shows an overview of significant main effects and two-variable interactions on each response. Each Y-variable defines a column containing either "NS" or + and - signs. The number of + and - signs in the plot indicates the degree of significance of the different effects, as detailed below.

Effects: significance limits

P-value	Negative effect	Positive effect
≥ 0.05	NS	NS
[0.01;0.05]	-	+
[0.001;0.01]	- -	+ +
<0.001	- - -	+ + +

The only choice you have to make on this sheet is which Significance Testing Method to use, which is selected from a drop-down menu.

The significant effects are found by comparing the effects with an estimate of the random variation. This random variation can be found in five different ways as displayed below, of which the first four choices are based on ordinary F-testing, with different error variance estimation:

Significance Testing Methods

Method	Description
Higher Order Interactions (HOIE)	This method assumes that all effects except those specified in the model (main effects or main effects plus interactions) are negligible. They are used in the error term for experimental error variance estimates.

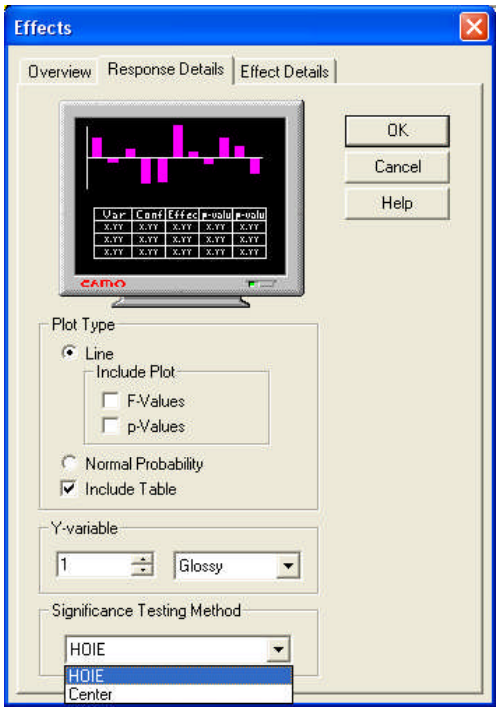
Center Samples	Replicates of the center samples are used to estimate the error.
Reference Samples	Replicates of the reference samples are used to estimate the error.
Center and Reference Samples	Replicates for both the center samples and the reference samples are used to estimate the experimental error.
COSCIND	A forward significance testing method starting with the smallest effect and stopping when an effect is declared as significant. The test statistics are related to the F-statistic in the first choice, but the p-values are computed in a stepwise fashion.

Only the significance testing methods that are appropriate for your data are shown in the drop-down list.

Effects Dialog: Response Details Sheet

The plot defined on this sheet shows the individual effects of the different variables and their interactions, for one response at a time. Choose between a plot of the individual effects as bars (Line Plot) or a Normal Probability Plot in the Plot Type field. The Line Plot presents the main effects of the design variables and their interactions as bars or a curve. F-values or p-values for checking significance of the effects can be added in separate windows. The Normal Probability Plot shows the effects versus the expected effect values under the assumption that all effects are normally distributed around zero. You can also choose to include a numerical table of the effects.

Dialog: Effects, Response Details sheet



Then, specify the Y-variable and select a Significance Testing Method from the drop-down list (for details on the methods, see the table in Effects Dialog: Overview Sheet).

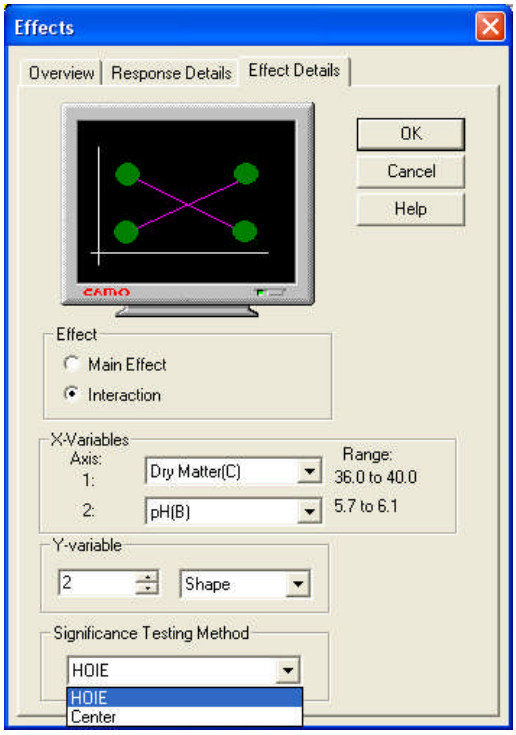
Effects Dialog: Effect Details Sheet

The plot defined on this sheet shows the Main Effect of a specific design variable or the Interaction between two design variables (X-variables), on one response at a time.

Choose between a plot of a Main Effect or an Interaction in the Effect field.

Select the X-variable(s) you want to display the effect of in the X-Variables field.

Dialog: Effects, Effect Details sheet



Then, specify the Y-variable to be plotted and select a Significance Testing Method from the drop-down list (for details on the methods, see the table in Effects Dialog: Overview Sheet).

Note:

In a fractional factorial design, the Interaction choice in the Effect field is greyed out if the interactions are confounded. Only interactions free of counfounding can be plotted.

Plot - Statistics

The **Statistics** dialog gives you access to all plots available after you have run a Statistics calculation. Select the tabbed sheet that gives you the information you are looking for. The available sheets are:

1. General;
2. Compressed;
3. Group (only available for designed data);
4. Scatter (only relevant for spectra);

5. Cross-Correlation (only available if you ticked the "Calculate Cross-Correlation" box in the Statistics dialog from Task - Statistics)

Statistics Dialog: General Sheet

On this sheet, you can specify individual plots of the types listed below, either for all samples or for pre-defined groups or subgroups of samples.

In the Plot field, you can choose between different plots, as displayed below:

Individual plot types

Plot type	Description
Mean	A plot of the average of each of the variables.
Standard Deviation	A plot of the standard deviation of each of the variables.
Mean and Std. Deviation	The mean is plotted as bars, with the standard deviation indicated by lines on top of the bars.
Percentiles	Shows the percentiles as a box plot.
Precision	A plot of the standard deviation of replicated samples is displayed.

Next, you choose whether you want to plot values for the different subgroups adjacent to each other (Line Plot), or generate a new dimension in the plot (Matrix Plot) for each different group in the field Plot Type, and in the Sample Groups field choose for which samples you want statistics to be run; Design Samples, Center Samples, Reference Samples or All Samples. The first three choices are only available for Statistics run on designed data. You can also select sample groups defined using levels of a category variable, or subgroups defined by the combinations of levels of several design variables.

Statistics Dialog: Compressed Sheet

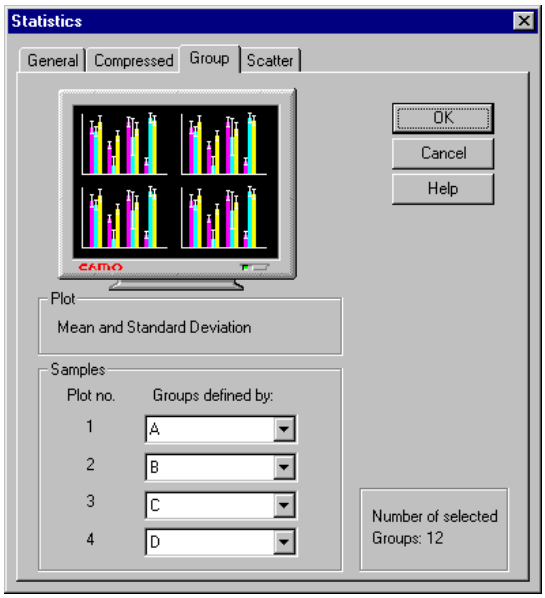
Here, you specify a double plot of the Percentiles (displayed as box-plot) and Mean and Standard Deviation (displayed as bars, indicating the standard deviation by lines on top of the bars). It is designed for simultaneous visualization of several features of location and variability of the data.

In the Sample Groups field, choose for which samples you want the statistics to be plotted: Design Samples, Center Samples, Reference Samples or All Samples. The first three choices are only available for Statistics run on designed data. You can also select sample groups defined using levels of a category variable, or subgroups defined by the combinations of levels of several design variables.

Statistics Dialog: Group Sheet

This dialog sheet is only available for Statistics results computed on designed data. You specify a quadruple plot showing four Mean and Standard Deviation plots, each with a number of groups defined by one of the design variables.

Dialog: Statistics, Group sheet



Decide which variable to use for sample grouping in each plot in the Samples field. The mean and standard deviation are computed for each level of the variables.

Statistics Dialog: Scatter Sheet

The plot you specify on this sheet is only relevant for Spectra. It shows the selected samples plotted against the average sample. Scatter effects are present if the slopes of the lines are different or if the baseline is changing from sample to sample, and are caused by e.g. different size of particles, opaque solutions, etc.. They can be removed with MSCorrection or differentiation.

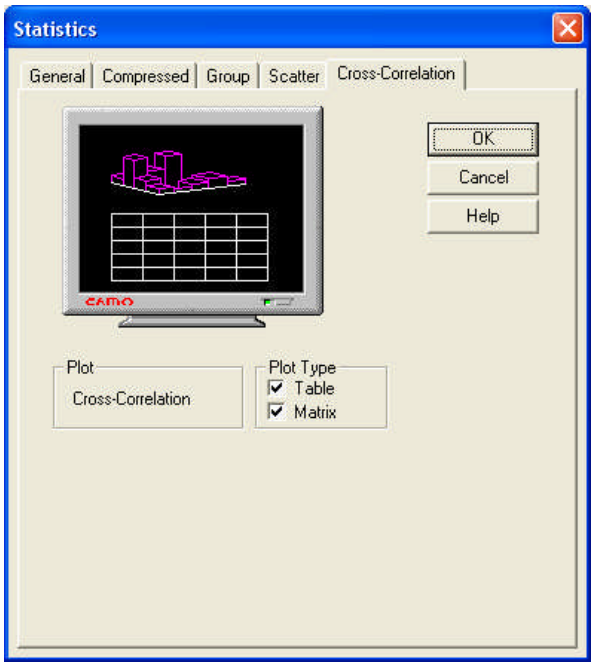
You only need to specify which samples are to be plotted this way in the Samples field.

Statistics Dialog: Cross-Correlation Sheet

This sheet allows you to display the cross-correlations among all variables in the analysis, either as a matrix plot or a table (or both).

By default, both boxes are ticked in the Plot Type field. If you wish to display only the matrix plot, un-tick the Table box and vice-versa. When displaying only one plot, you may double-click on the Plot Preview to select a single-subview viewer.

Dialog: Statistics, Cross-Correlation sheet



The default layout for the matrix plot of cross-correlations is “Bars”, as shown in the plot preview. Once the plot is displayed (after you clicked OK), you may change the layout if you wish, by using **Edit - Options** or or **Ctrl+L**.

Plot - Classification

Plots that are specific to classifications are plotted from the **Classification** dialog. The different plots available in the dialog are displayed below.

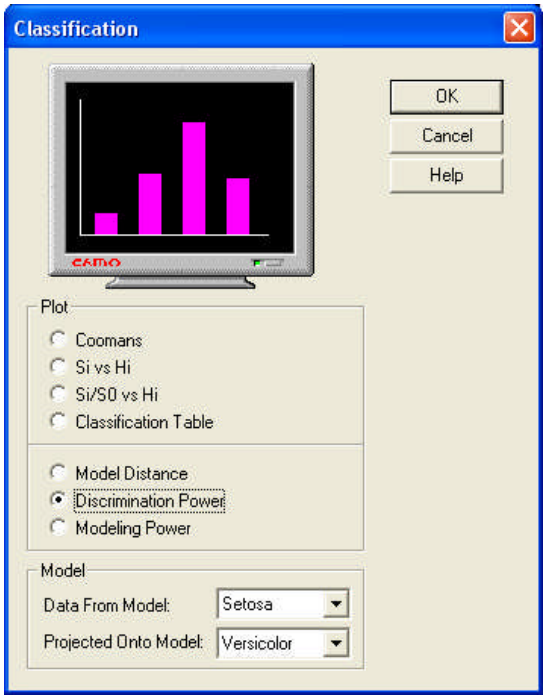
Classification plots

Type	Description
Coomans	Shows the orthogonal distances from the new objects to two different models at the same time
Si vs Hi	Shows the limits used for classification; both distance to model (residual standard deviation) and leverage (distance to model center)
Si/H0 vs Hi	The same as Si vs Hi, but the distance measures are relative to the average distance in the model
Classification Table	Shows compressed numeric results for each classified sample
Model Distance	Shows the distances between different models
Discrimination Power	Shows how much the different variables contribute to separating different models
Modeling Power	Shows how much the variables contribute to the model

All of these plots except the Classification Table require that you select the model for which you want to see the **Classification** results from the drop-down menu Data From Model in the Model field. Discrimination

Power and Classification plots involve two models; select the second model from the drop-down menu at the bottom.

Dialog: Classification



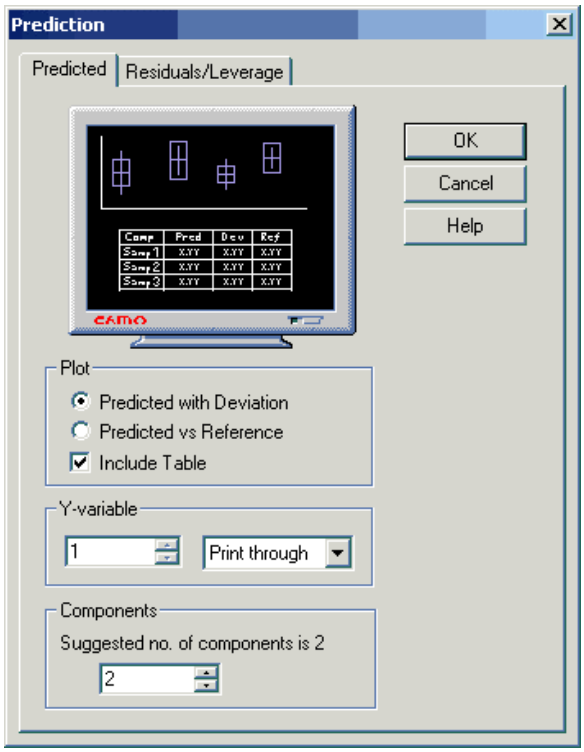
Plot - Prediction

The **Prediction** dialog lets you plot the predicted values from a prediction or the residuals and leverage of the predicted samples from two different sheets: Predicted and Residuals/Leverage.

Prediction Dialog: Predicted Sheet

On this sheet you can define a plot of the predicted Y-values from a regression analysis.

Prediction Dialog, Predicted Sheet



You can choose between two different plots in the Plot field:

1. Predicted with Deviation, which shows the predicted values with an estimate of the uncertainty (deviation) connected with the prediction of each sample;
2. Predicted vs Reference, which plots the predicted values versus the reference values. The reference values were included for comparison purposes when you made the predictions.

Note: Deviations are used to identify outliers, and nothing else. Do not use them e.g. to express the prediction error.

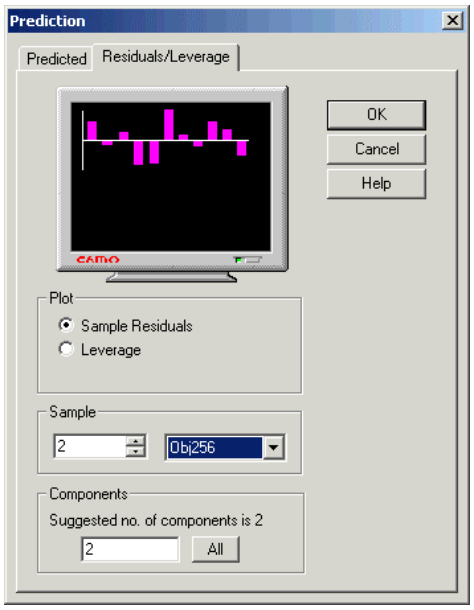
In the Plot field, you can also choose to include a table which contains the predicted value, the deviation, and the reference value of each sample in the prediction. You cannot select several components when this option is selected.

Select the Y-variable for which you want to look at the predictions and choose how many components to use in the prediction in the appropriate fields. You should use the optimal number of components you found for the model based on validation.

Prediction Dialog: Residuals/Leverage Sheet

From this dialog sheet, you can specify a plot of prediction residuals or of the leverage for the prediction samples. Those two elements participate in building the Deviations. Use the plots to understand why some samples have larger deviations than the others.

Prediction Dialog, Residuals/Leverage Sheet



In the Plot field, choose whether you want to plot Sample Residuals, which show the X-residuals of the samples after the specified number of components have been extracted from the data, or Leverage, which shows the leverage of each sample.

If you choose Sample Residuals, you must also choose which sample to look at in the Sample field, and in both cases, you must choose how many components to use in the prediction. You should use the optimal number of components you found for the model based on validation.

Plot - Line (General View)

This command, selected from the General Viewer, launches a dialog where you can specify a ***line plot*** of any vector of your choice, from any Unscrambler file.

Select the file from which you want to plot in the Source field.

If you do not remember the file name, click the Browse button to launch the **Results** dialog, described in **Results - All…**. There, you can search for the right file. Press Select to insert the correct file name in the dialog.

Source File Is A Data Table

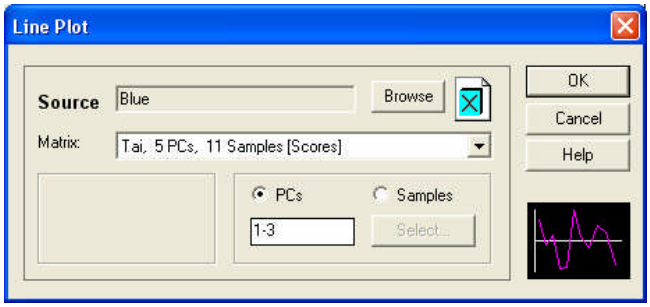
Once you have selected a source, you must specify whether to plot ***samples*** or ***variables*** in the bottom right field. Then, select which sample(s) or variable(s) to plot, either by entering it directly or by pressing Select to enter an Editor where you can mark your selection. Ranges are indicated by a hyphen, ranges or separate items are separated by a comma.

Source File Is A Result File

In this case, you must specify from which ***matrix*** stored in the result file you wish to plot. Then, select which dimension of the matrix you wish to pick elements from; the dimension which you have not selected is the one that will vary in the plot.

For instance, in the figure below, the source file is a **PCA result file** called "Blue". The selected matrix is the **scores matrix Tai**, and **PCs number 1-3** are selected, which means that three lines will be plotted. The plotted elements for the first line are the scores along PC1 for the 11 samples, for the second line: along PC2, and for the third line: along PC3.

Dialog: Line Plot in General View



Note: You may select more than one vector at a time; each vector will appear as a separate line on the plot.

In the bottom right corner of the dialog, a preview screen shows how the plot will look in the General View.

Note: The preview plot is a general example and does not show what your actual data look like.

Once the plot is displayed in the General Viewer, you may add more lines with the command **Edit - Add Plot**. This opens a new dialog where you can select more vectors to be plotted together with the ones already displayed.

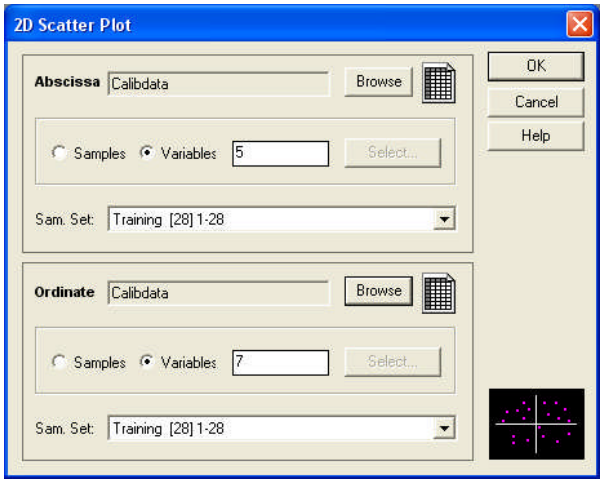
Plot - 2D Scatter (General View)

This option launches the **2D Scatter Plot** dialog.

First, you must specify the file which you want to plot as ***abscissa*** (horizontal axis) in the Abscissa field, and the one you want to plot as ***ordinate*** (vertical axis) in the Ordinate field.

If you do not remember the file name(s), click the Browse button in the field(s) in question to launch the **Results** dialog, described in **Results - All…**. There, you can search for the right file. Press Select to insert the correct file name in the **2D Scatter Plot** dialog.

Dialog: 2D Scatter Plot in General View



Source File Is A Data Table

Once you have selected a source, you must specify whether to plot a selected ***sample*** or ***variable*** along the abscissa and the ordinate. Then, select which variable set or sample set to take into account.

For instance, in the dialog example shown in the above figure, the same **data file** "Calibdata" has been chosen as source for Abscissa and Ordinate. The vectors to be plotted against each other are **variables number 5 and 7**. The samples (which will appear as points on the plot) are taken from **sample set** "Training".

Source File Is A Result File

In this case, you must specify from which ***matrix*** stored in the result file you wish to plot your Abscissa vector, and from which to plot your Ordinate vector. Then, select which dimension of the matrix you wish to pick elements from; the dimension which you have not selected is the one that will vary in the plot.

Note: You may select more than one vector at a time as Abscissa or Ordinate (or both); each couple of vectors will appear as a separate series of points on the plot.

Once the plot is displayed in the General Viewer, you may add more series of points with the command **Edit - Add Plot**. This opens a new dialog where you can select more vectors to be plotted together with the ones already displayed.

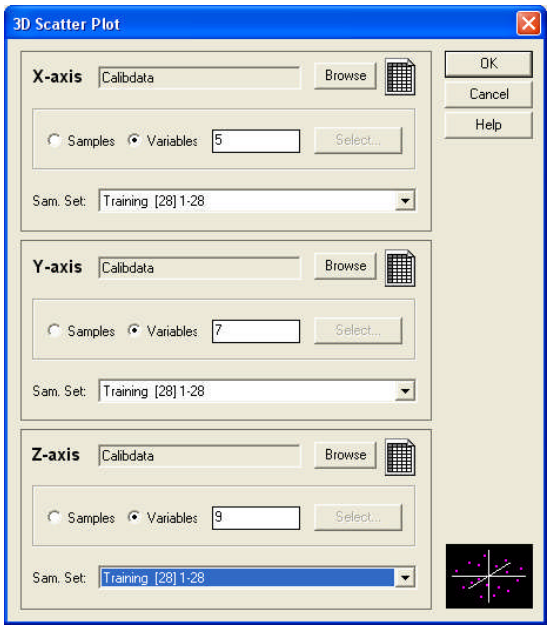
Plot - 3D Scatter (General View)

This option launches the **3D Scatter Plot** dialog.

Here, you must specify the file which you want to plot as X, Y and Z in the X-, Y- and Z-axis fields.

If you do not remember the file name(s), click the Browse button in the field(s) in question to launch the **Results** dialog, described in **Results - All...**. There, you can search for the right file. Press Select to insert the correct file name in the **3D Scatter Plot** dialog.

Dialog: 3D Scatter Plot in General View



Source File Is A Data Table

Once you have selected a source, you must specify whether to plot a selected ***sample*** or ***variable*** along the X, Y and Z axes. Then, select which variable set or sample set to take into account.

For instance, in the dialog example shown in the above figure, the same **data file** "Calibdata" has been chosen as source for X, Y and Z. The vectors to be plotted against each other are **variables number 5, 7 and 9**. The samples (which will appear as points on the plot) are taken from **sample set** "Training".

Source File Is A Result File

In this case, you must specify from which ***matrix*** stored in the result file you wish to plot your X vector, Y vector and Z vector. Then, select which dimension of the matrix you wish to pick elements from; the dimension which you have not selected is the one that will vary in the plot.

Note: You may select more than one vector at a time as X, Y or Z (or all); each triplet of vectors will appear as a separate series of points on the plot.

Once the plot is displayed in the General Viewer, you may add more series of points with the command **Edit - Add Plot**. This opens a new dialog where you can select more vectors to be plotted together with the ones already displayed.

Plot - Histogram (General View)

This command, selected from the General Viewer, launches a dialog where you can specify a ***histogram plot*** of any vector of your choice, from any Unscrambler file.

Select the file from which you want to plot in the Source field.

If you do not remember the file name, click the Browse button to launch the **Results** dialog, described in **Results - All…**. There, you can search for the right file. Press Select to insert the correct file name in the dialog.

Source File Is A Data Table

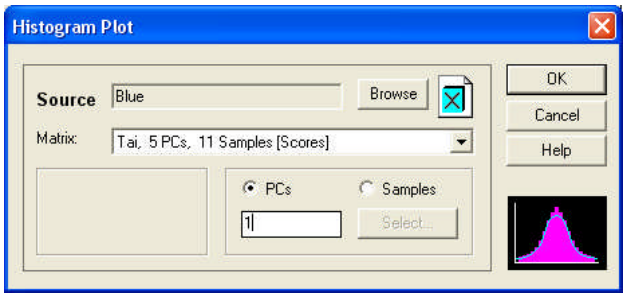
Once you have selected a source, you must specify whether to plot ***samples*** or ***variables*** in the bottom right field. Then, select which sample(s) or variable(s) to plot, either by entering it directly or by pressing Select to enter an Editor where you can mark your selection. Ranges are indicated by a hyphen, ranges or separate items are separated by a comma.

Source File Is A Result File

In this case, you must specify from which ***matrix*** stored in the result file you wish to plot. Then, select which dimension of the matrix you wish to pick elements from; the dimension which you have not selected is the one that will vary in the plot.

For instance, in the figure below, the source file is a **PCA result file** called "Blue". The selected matrix is the **scores matrix Tai**, and **PC number 1** is selected, which means that the plotted elements are the scores along PC1 for the 11 samples.

Dialog: Histogram Plot in General View



Note: Only one vector at a time can be plotted as histogram.

In the bottom right corner of the dialog, a preview screen shows how the plot will look in the General View.

Note: The preview plot is a general example and does not show what your actual data look like.

Plot - Matrix (General View)

This command, selected from the General Viewer, launches a dialog where you can specify a ***plot*** of any ***matrix*** of your choice, from any Unscrambler file.

Select the file from which you want to plot in the Source field.

If you do not remember the file name, click the Browse button to launch the **Results** dialog, described in **Results - All...**. There, you can search for the right file. Press Select to insert the correct file name in the dialog.

Source File Is A Data Table

Once you have selected a source, you must specify whether to plot ***samples*** or ***variables*** in the bottom right field. Then, select which sample(s) or variable(s) to plot, either by entering it directly or by pressing Select to enter an Editor where you can mark your selection. Ranges are indicated by a hyphen, ranges or separate items are separated by a comma.

Source File Is A Result File

In this case, you must specify which ***matrix*** stored in the result file you wish to plot.

Note1: Only one matrix can be plotted at a time.

Note2: Only a whole matrix can be plotted.

In the bottom right corner of the dialog, a preview screen shows how the plot will look in the General View.

Note: The preview plot is a general example and does not show what your actual data look like.

Plot - Normal Probability (General View)

This command, selected from the General Viewer, launches a dialog where you can specify a ***normal probability plot*** of any vector of your choice, from any Unscrambler file.

Select the file from which you want to plot in the Source field.

If you do not remember the file name, click the Browse button to launch the **Results** dialog, described in **Results - All…**. There, you can search for the right file. Press Select to insert the correct file name in the dialog.

Source File Is A Data Table

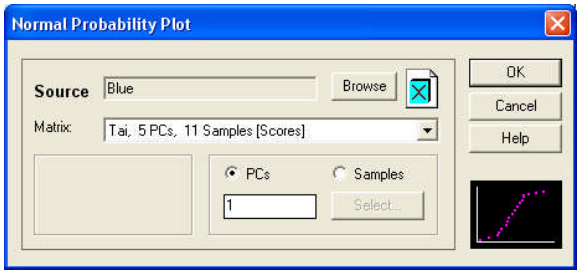
Once you have selected a source, you must specify whether to plot ***samples*** or ***variables*** in the bottom right field. Then, select which sample(s) or variable(s) to plot, either by entering it directly or by pressing Select to enter an Editor where you can mark your selection. Ranges are indicated by a hyphen, ranges or separate items are separated by a comma.

Source File Is A Result File

In this case, you must specify from which ***matrix*** stored in the result file you wish to plot. Then, select which dimension of the matrix you wish to pick elements from; the dimension which you have not selected is the one that will vary in the plot.

For instance, in the figure below, the source file is a **PCA result file** called "Blue". The selected matrix is the **scores matrix Tai**, and **PC number 1** is selected, which means that the plotted elements are the scores along PC1 for the 11 samples.

Dialog: Normal Probability Plot in General View



Note: Only one vector at a time can be plotted as normal probability plot.

In the bottom right corner of the dialog, a preview screen shows how the plot will look in the General View.

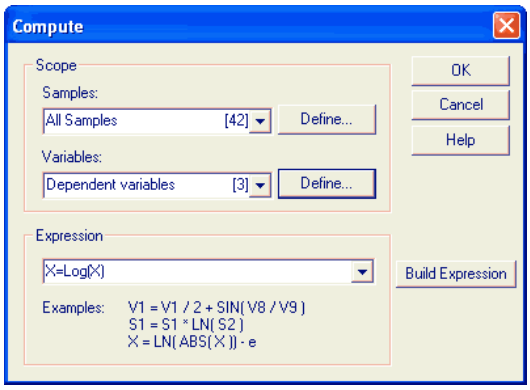
Note: The preview plot is a general example and does not show what your actual data look like.

The Modify Menu

Modify - Compute General

Access this option from menu **Modify - Compute General** or by clicking on the corresponding shortcut item in the Main Editor Toolbar. This brings you to the **Compute** dialog, which lets you perform arithmetic and more advanced computations on the whole data table or on selected samples or variables. This option also helps in transforming variables.

Dialog: Compute



In the Scope field, select the Sample and Variable Sets to be affected by the computation. Click Define… if you need to define a new set; this will take you to the **Set Editor**.

There are three ways of defining the mathematical expression to be applied. You may:

1. Type your expression directly in the Expression box,
2. Use the drop-down list, which gives you access to the latest used expressions (if this is the first time you are using the **Compute** dialog, no formerly used expressions will show in the drop-down list).
3. Click on the Build Expression button. This takes you to the **Build Expression** dialog wherein you can build your expression using the ready-made functions and operators allowed in The Unscrambler.

The Expression box accepts the expression as a formula of the type: **"X=LN(ABS(X))-e" or "S4=(S1*S2)+S3" or "V1=V1/2+SIN(V8/V9)"**

where S stands for sample, V stands for variable, and the number is the sample or variable number in the Editor. To build general expressions that are not related to a particular sample or variable, use "X". "X" stands for the whole matrix defined by the variable and sample set chosen in Scope.

Note: The formula cannot contain mixed references to samples (S), variables (V) and X.

The constants, operators, and functions that are allowed in computations are listed below:

Table: Constants, operators and functions allowed in computations

Name	Description	Name	Description
PI	3.14	ATAN2(X1, X2)	Arcus tangent
e	2.718	COS(X)	Cosine
+	Addition	COSH(X)	Hyperbolic cosine
-	Subtraction	EXP(X)	Exponential(X)=e^X
*	Multiplication	LN(X)	Natural logarithm (base e)
/	Division	LOG(X)	Briggs logarithm (base 10)
=	Equals to	MAX(X1, X2, ...)	Maximum value
^	Power	MIN(X1, X2, ...)	Minimum value
(	Left Parenthesis	SIGN(X)	-1 if X < 0, 1 if X >= 0
)	Right Parenthesis	SIN(X)	Sine
ABS(X)	Absolute value of X	SINH(X)	Hyperbolic sine
ACOS(X)	Arcus cosine (radians)	SQRT(X)	Square root of X
AINT(X)	Integer part of X	TAN(X)	Tangent
ANINT(X)	Nearest integer (rounding)	TANH(X)	Hyperbolic tangent
ASIN(X)	Arcus sine (radians)		

“X” can denote both samples and variables in this table.

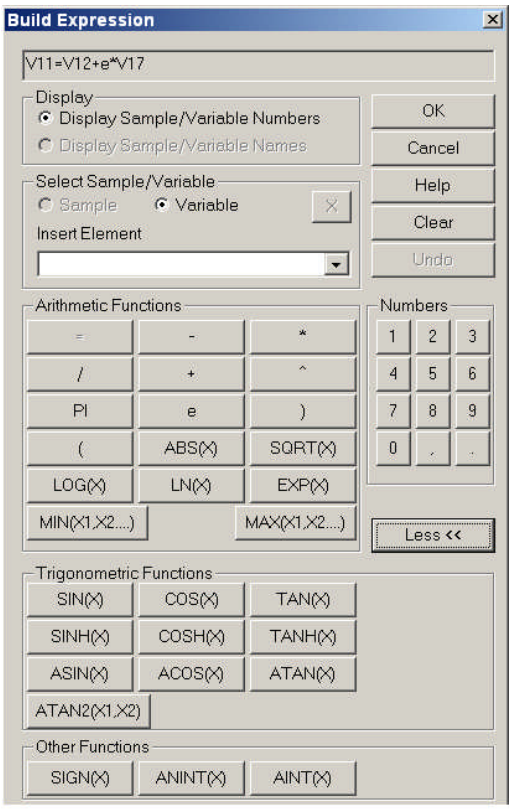
Note1: A commonly used expression is **X=Log(X)**. This expression generally transforms skewed variable distributions into more symmetrical ones. Use a histogram plot or Variable Statistics in order to check whether the skewness was improved or deteriorated after applying the transformation.

Note2: You may Undo / Redo operations performed in the **Compute** dialog with the corresponding options in the **Modify** menu.

Build Expression Dialog

In the **Build Expression** dialog you can build your expression using the ready-made functions and operators allowed in The Unscrambler.

Dialog: Build Expression



The upper text field shows the expression as it is being built. In Display, choose whether you want the text field to show the sample/variable Numbers or the sample/variables Names. In the Insert field, choose to insert specific samples, specific variables or X (general expression). If you choose the Sample or the Variable options, the drop-down list is enabled and you may select the relevant object(s) from the list. The available samples or variables are only those belonging to the Scope formerly selected in the **Compute** dialog.

Note: The formula cannot contain mixed references to samples (S), variables (V) and X.

The Arithmetic Functions, Trigonometric Functions, Other Functions and Numbers fields offer buttons and are used in the same principle as for a calculator. The More>> and Less<< buttons let you expand/reduce the number of available functions.

Click Clear to refresh the expression. Click Undo to undo the latest insertion in the expression text. Clicking OK brings you back to the **Compute** dialog.

Modify - Transform

With this option you can transform your samples or variables to get data properties which are more suitable for analysis and easier to interpret. Bilinear models, e.g. PCA and PLS, basically assume linear data. The transformations should therefore result in a more symmetric distribution of the data and a more linear behavior, if you have non-linearities.

Note: Transformations which may change the dimensions of your data table are disabled for 3-D data tables.

The Unscrambler contains many standard transformations, to be found as sub-options in **Modify - Transform**, but you can also take advantage of the **Modify - Compute General** function to transform the data with simple formulas (e.g. logarithm).

Here are all the choices to be found under the **Modify - Transform** menu option:

- Modify - Transform - Smoothing - Moving Average
- Modify - Transform - Smoothing - Savitzky-Golay
- Modify - Transform - Smoothing - Median Filter
- Modify - Transform - Smoothing - Gaussian Filter
- Modify - Transform - Normalize
- Modify - Transform - Spectroscopic Transformation
- Modify - Transform - MSC
- Modify - Transform - Noise
- Modify - Transform - Derivatives - Norris Gap
- Modify - Transform - Derivatives - Gap-Segment
- Modify - Transform - Derivatives - Savitzky-Golay
- Modify - Transform - Baseline
- Modify - Transform - SNV
- Modify - Transform - Center and Scale
- Modify - Transform - Reduce (Average)
- Modify - Transform - Transpose
- Modify - Transform - User-defined

Modify - Transform - Smoothing

Smoothing is used to reduce the noise in the data without reducing the number of variables. It is a row-oriented transformation, that is to say the contents of a cell are likely to be influenced by its horizontal neighbors.

A sub-menu to the **Smoothing** menu lets you choose between four different methods to smooth your data:

1. **Moving Average** first finds a data value by averaging the values within a segment of data points;
2. **Savitzky-Golay** finds a data value by making a polynomial to fit the data points using a number of data points on each side;
3. **Median Filter** finds a data value by taking the median within a segment of data points;
4. **Gaussian Filter** finds a data value by computing a weighted moving average within a segment of data points.

Modify - Transform - Smoothing - Moving Average

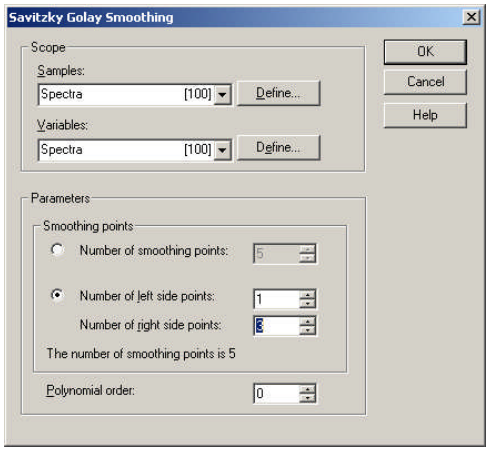
In the **Moving Average Smoothing** dialog, you can replace each value in a row by the average of its nearest neighbors.

First, select the sample and variable sets that define the matrix you want to smooth in the Scope field. The Define buttons in the Scope field launches the **Set Editor**, where you can define new sample and/or variable sets. Then, you enter the size of the segment to be averaged, i.e. how many adjacent columns should be used to compute the average value, in the Parameters field.

Modify - Transform - Smoothing - Savitzky-Golay

Savitzky-Golay is an averaging algorithm that fits a polynomial to the data points. The value to be averaged is then predicted from this polynomial equation.

Dialog: Savitzky-Golay Smoothing



In the Scope field in the **Savitzky-Golay Smoothing** dialog, select the Sample and variable sets that define the matrix you want to smooth. If necessary, use the Define buttons to enter the **Set Editor** and define new sets.

You may then select the smoothing points in the Parameters field. Note that a larger range will give a smoother shape to the sample, but you may lose some information. There are two ways of selecting the smoothing points:

- Either type in the Number of smoothing points - it is always an odd number 2n + 1, and the smoothing segment will be symmetrically distributed on both sides of each curve point (n left side points, n right side points),
- Or choose the Number of left side points and right side points separately.

Finally, enter the order of the polynomial to be fitted in the sub-field Polynomial Order. For instance, a polynomial order of 2 means that a second-degree equation will be used to fit the data points.

Note that, after the operation is completed, the data will be slightly truncated at both ends. If *p* is the number of left side points and *q* the number of right side points in the smoothing segment, the first *p* and the last *q* variables in the smoothed variable set will be set to zero. This is because there are not enough points to the left (resp. right) of these variables to compute the smoothing function.

Modify - Transform - Smoothing - Median Filter

In the **Median Filter Smoothing** dialog, you can replace each value in a row by the median of the values within a given segment centered on the point to be smoothed.

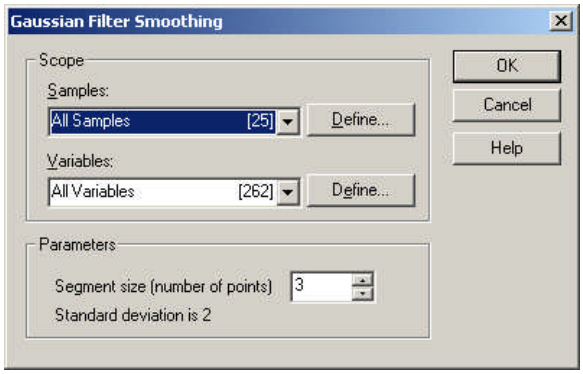
First, select the sample and variable sets that define the matrix you want to smooth in the Scope field. The Define buttons in the Scope field launches the **Set Editor**, where you can define new sample and/or variable sets. Then, you enter the size of the segment to be smoothed, i.e. how many adjacent columns should be used to compute the median, in the Parameters field.

Note: The Median Filter is supported in auto-pretreatments.

Modify - Transform - Smoothing - Gaussian Filter

In the **Gaussian Filter Smoothing** dialog, you can replace each value in a row by a fitted value determined by a Gaussian filter function of its nearest neighbors. In practice, this amounts to averaging values within a segment of data points that have been weighted according to a Gaussian distribution function with $\sigma^2 = 2$.

Dialog: Gaussian Filter Smoothing



First, select the sample and variable sets that define the matrix you want to smooth in the Scope field. The Define buttons in the Scope field launches the **Set Editor**, where you can define new sample and/or variable sets.

Then, you enter the size of the segment to be used for smoothing, i.e. how many adjacent columns should be used to compute the gaussian fitted value, in the Parameters field.

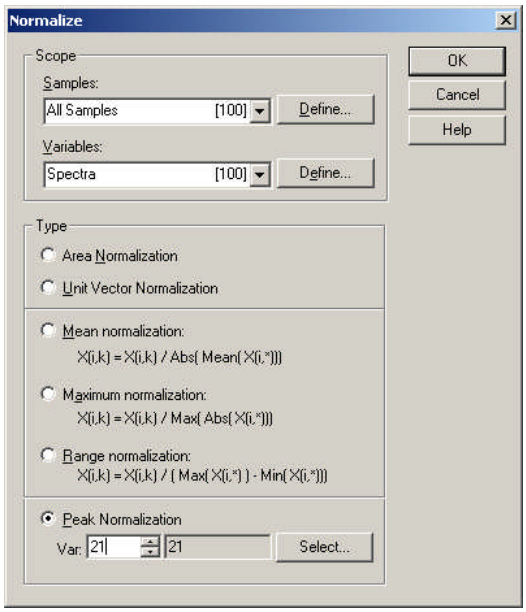
Note: The Gaussian Filter is supported in auto-pretreatments.

Modify - Transform - Normalize

Normalization is used to get all data in approximately the same scaling, or to get a more even distribution of the variances and the average values. It is a row-oriented transformation, that is to say the contents of a cell are likely to be influenced by its horizontal neighbors.

Chromatography data are usually normalized before analysis.

Dialog: Normalize



In the Scope field in the **Normalize** dialog, select the sample and variable sets that define the matrix you want to normalize. If necessary, select Define to enter the **Set Editor** and define new sets.
Then, select the normalization type in the Type field. These 6 normalization methods are available:

1. **Area normalization**
   Area normalization attempts to correct the spectra for indeterminate path length when there is no way of measuring it, or isolating a band of a constant constituent. The transformation normalizes a spectrum X_i by calculating the area under the curve for the spectrum.
2. **Unit vector normalization**
   Unit vector normalization normalizes sample-wise data X_i to unit vectors. It can be used for pattern normalization, which is useful for pre-processing in some pattern recognition applications.
3. **Mean normalization**
   Mean normalization is the standard normalization that is used within chromatography. The areas below the spectra are made equal. The results of a Mean normalization on two different samples are listed below.

Result of a Mean normalization on two different samples

Before				After			
1	2	3	4	0.4	0.8	1.2	1.6
2	4	6	8	0.4	0.8	1.2	1.6

4. **Maximum normalization**
   Maximum normalization is a normalization that “polarizes” the spectra. The peaks of all spectra with positive values touch +1, while spectra with values of both signs touch -1.
5. **Range normalization**
   Range normalization involves scaling all samples to a common range, for example between 0 and +1. Thus each axis in a plot of range-scaled data is adjusted such that the data fill the region of the plot in all directions. The results of a Range normalization on two different samples are listed below.

Result of a Range normalization on two different samples

Before							After						
10	25	30	25	10	5	3	0.33	0.83	1.00	0.83	0.33	0.16	0.10
0.3	0.5	1.0	2.5	3.0	2.5	1.0	0.10	0.16	0.33	0.83	1.00	0.83	0.33

6. **Peak normalization**
   Peak normalization normalizes a sample as the ratio of each value by the value at a selected spectral point (or wavelength). The chosen spectral point (usually the maximum peak of a band of the constant constituent, or the isosbestic point) is assumed to be concentration invariant in all samples.
   Type in the number of the peak variable in field Var:, or use the Select button to select the peak variable directly from an Editor window.

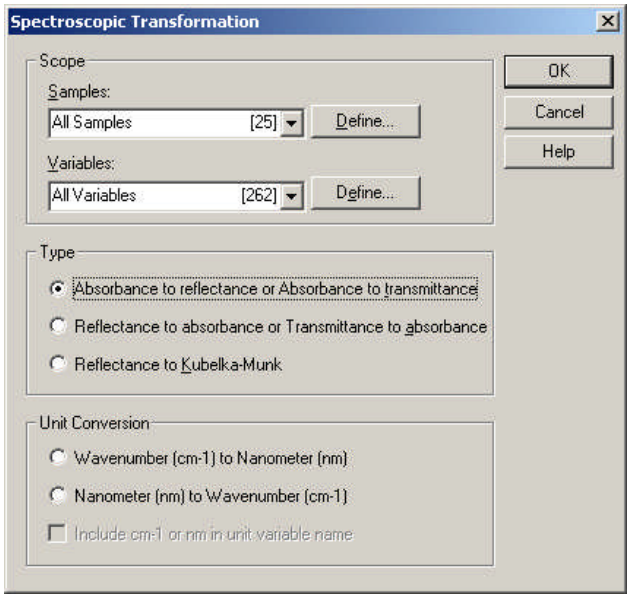
Note: If you peak-normalize your calibration samples before building a model for later use in prediction or classification, make sure that ***the same peak variable*** is selected when you normalize the prediction samples!

The equations used to normalize the samples are listed in the Method References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices.

Modify - Transform - Spectroscopic Transformation

Sometimes you want to transform your spectra from one format to another. **Spectroscopic transformations** let you switch between absorbance and reflectance data and transform reflectance data into Kubelka-Munk units.

Dialog: Spectroscopic Transformation



In the **Spectroscopic Transformation** dialog, select the sample and variable sets that define the matrix you want to transform in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets. Then, select the transformation type in the next fields.

Three types of transformations can be performed on the ***data values***, using the options from frame Type:

1. Absorbance to reflectance
   Absorbance to transmittance;
2. Reflectance to absorbance
   Transmittance to absorbance;
3. Reflectance to Kubelka-Munk.

As for the frame Unit Conversion, it allows you to convert the units for the ***variable names*** by shifting from Wavenumber (cm-1) to Nanometer (nm) and vice versa. Tick the box at the bottom if you wish to include cm-1 or nm in unit variable name.

Note 1: The unit conversion option is disabled if the selected variable set has names all " * " or strings.

Note 2: Unit conversion is *not* supported as an automatic pre-treatment.

If some of the variable names cannot be interpreted as wavenumbers or wavelengths, the following error message is displayed when attempting Unit Conversion:

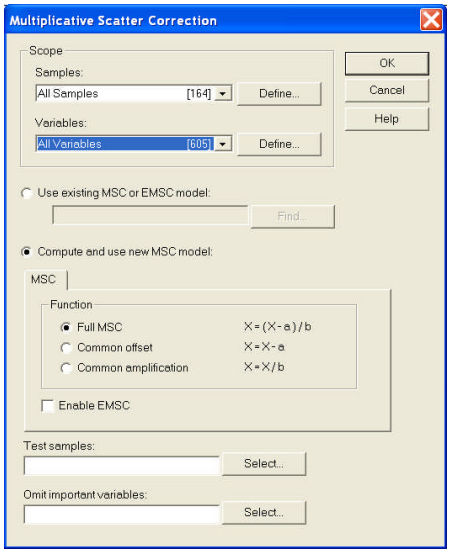
The Unscrambler
One or more variable names were not recognized as possible wavenumbers and wavelengths. Unit Conversion applies on numerical values for wavenumbers or wavelengths.
OK

and the conversion is not performed.

Modify - Transform - MSC/EMSC

MSCorrection is a transformation method used to compensate for multiplicative and/or additive scatter effects in the data. **EMSCorrection** is an extension to regular MSCorrection using prior knowledge that includes extra parameters that can account for the physical or chemical phenomena that affected the spectra. Both methods are row-oriented transformations, that is to say the contents of a cell are likely to be influenced by its horizontal neighbors.

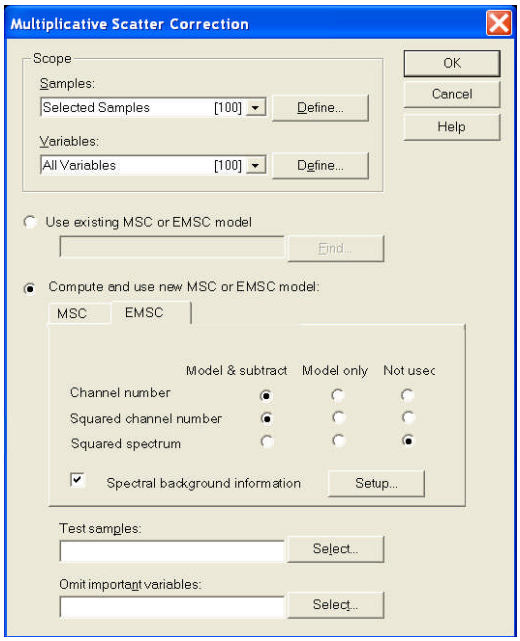
Dialog: Multiplicative Scatter Correction



In the **Multiplicative Scatter Correction** dialog, select the Sample and variable sets that define the matrix you want to correct in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets. Then, click the radio button Use existing MSC or EMSC Model if you want to be able to read an MSC or EMSC model from a file to transform your current data in exactly the same way as you did for an earlier data table. This is useful if you want to treat different data tables in the same way, e.g. new prediction samples. Press the Find button to enter the **Open File** dialog if you do not remember the name of the MSC or EMSC model.

The default choice is to Compute and use new MSC or EMSC model by clicking this radio button. You must then decide whether to make a full MSC model, common offset (additive effects) model, or common amplification (multiplicative effects) model in the Function field. In addition to regular MSC, you can also activate EMSC by clicking the check box Enable EMSC. An extra tab becomes visible, indicating the available options in EMSC.

Dialog: Multiplicative Scatter Correction with EMSC options field



When EMSC is enabled, you must decide which effects to include. The options Channel number and Squared channel number model physical effects related to wavelength dependent light scatter variations. Chemical effects are included in Squared spectrum. For all three options, you can choose Not used, and the effect will not be included in the transformation. If Model only is selected, the effect will be included to calculate EMSC parameters. By clicking Model & subtract, the effect will not only be included, but the effect will also be subtracted from the EMSC corrected spectra.

It is also possible to include available background spectra in the EMSC calculation by clicking the check box Spectral background information and then clicking on Setup to enter the **Background information setup** dialog.

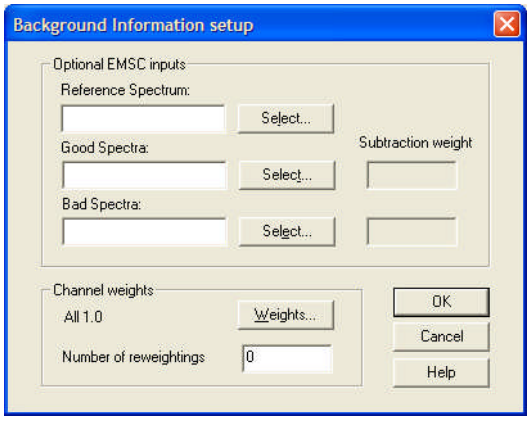
In the Test Samples field, you also have to specify the test samples you are going to include in your test set validation in later analyses. These samples are not used to find the correction factors, but they are MSC or EMSCorrected the same way as the other samples. Finally, specify the variable ranges that contain chemical information, i.e. not background noise, to omit those. You may enter several ranges of variables that are not continuous. Pressing the Select button next to any of the two last fields will launch the **Select**

Samples/Select Variables dialog respectively, which displays an Editor where you can make your selection directly.

MSC/EMSC: Background information setup Dialog

This dialog is accessed by clicking Setup after you chose Spectral background information in the **Multiplicative Scatter Correction** dialog. It allows you to provide the EMSC model with prior knowledge about your data.

Dialog: Background information setup



The Reference Spectrum field gives you the opportunity to select a single spectrum from your data acting as a typical spectrum without any additional effects. If not selected, a reference will be calculated using the mean of all spectra. In the Good Spectra and the Bad Spectra fields, you can specify several spectra from your data table that you believe are good and bad representatives of your spectral data, respectively. If you have selected data in the Good Spectra and the Bad Spectra fields, you are also allowed to enter a subtraction weight for the respective spectra. These subtraction weights are multiplied to the good and the bad spectra and subtracted from the corrected spectra.

It should also be noted that the background spectra available for selection in the Select… button are those contained within the variable Scope defined in the **Multiplicative Scatter Correction** dialog. This is due to the fact that spectra used as background spectra must have the same number of variables as the spectra to be transformed. It is also recommended that you select background spectra to be different samples from the samples in the selected scope of your data table. Overlapping reference, good and bad spectra is not allowed. A warning message will appear if this happens.

Example:

Let us say that your data table consists of several spectra measured on different **mixtures of two chemical compounds** where the amount of each of the two substances is varying.

The **reference** spectrum can be a spectrum measured on a mixture where the two compounds are ***equally represented***.

Good spectra would then be spectra measured on ***each compound alone***.

The **bad spectra** could then be selected as spectra believed to contain ***additional effects***, not caused by the chemicals.

The last entry in the **Background information setup** dialog is the Channel Weights field. Here, you can choose to select different weighting of your variables. It is also possible to iteratively find better weights than the default choice, by entering a number in the Number of reweightings field. The EMSC will then be run this number of times to find improved weights.

Modify - Transform - Noise

You can introduce additive and/or proportional noise into the selected data range. This may be useful to see how sensitive your model is to noise in the data. This transformation has no specific row- or column orientation, that is to say you can compute the new value of a cell independently from its neighbors.

In the **Noise** dialog, select the sample and variable sets that define the matrix you want to correct in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets. Then, in the Parameters field, specify the level of proportional noise (e.g. 5%) and the standard deviation of the additive noise you want to add.

Modify - Transform - Derivatives

Differentiation, i.e. computing derivatives of various orders, is a classical technique widely used for spectroscopic applications. Some of the information "hidden" in a spectrum may be more easily revealed when working on a first or second derivative. It is a row-oriented transformation, that is to say the contents of a cell are likely to be influenced by its horizontal neighbors.

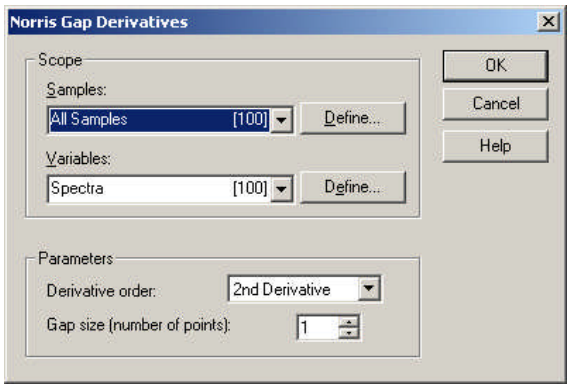
Three algorithms are available for computing derivatives:

1. Norris Gap;
2. Gap-Segment;
3. Savitzky-Golay.

Modify - Transform - Derivatives - Norris Gap

This method computes derivatives of up to the 4th order. It has the advantage of not generating any missing value at the ends of the spectrum.

Dialog: Norris Gap Derivatives



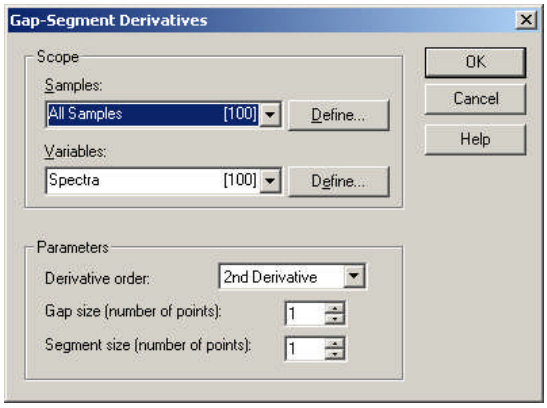
In the Scope field, select the samples and variables to be transformed. If necessary, press Define to enter the **Set Editor** and define new sets.

In the Parameters field, choose the Derivative order, i.e. whether you want the 1st, 2nd, 3rd, or the 4th derivative of the samples, from the drop-down list. Then, select the required Gap size (width of the interval between the two values used for differentiation).

Modify - Transform - Derivatives - Gap-Segment

This method computes derivatives of up to the 4th order. It is a more complex version of the Norris gap method that includes an additional segment option for smoothing.

Dialog: Gap-Segment Derivatives



In the Scope field, select the samples and variables to be transformed. If necessary, press Define to enter the **Set Editor** and define new sets.

In the Parameters field, choose the Derivative order, i.e. whether you want the 1st, 2nd, 3rd, or the 4th derivative of the samples, from the drop-down list. Then, select the required Gap size and Segment size.

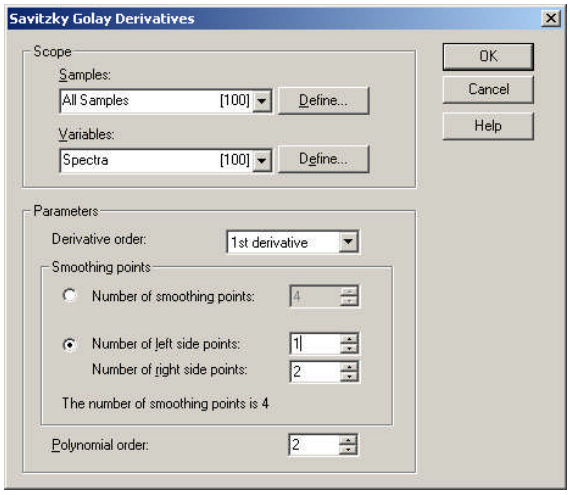
Note:

- The segment size must be an odd number for 2nd or 4th derivative.
- The gap size must be an odd number for 1st or 3rd derivative.

Modify - Transform - Derivatives - Savitzky-Golay

Savitzky-Golay differentiation computes derivatives of up to the 4th order, based on a polynomial approximation of a portion of the curve.

Dialog: Savitzky-Golay Derivatives



Make the appropriate choices in the **Savitzky Golay Derivatives** dialog by first selecting the sample and variable sets that define the matrix you want to differentiate in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets.

In the Parameters field, choose the Derivative order, i.e. whether you want the 1st, 2nd, 3rd, or the 4th derivative of the samples, from the drop-down list.

You may then select the smoothing points. Note that a larger range will give a smoother shape to the sample, but you may lose some information. There are two ways of selecting the smoothing points:

- Either type in the Number of smoothing points - it is always an odd number 2n + 1, and the smoothing segment will be symmetrically distributed on both sides of each curve point (n left side points, n right side points),
- Or choose the Number of left side points and right side points separately.

Enter how many variables (data points) should be taken into account on the left and right side of each cell in the Averaging sub-field.

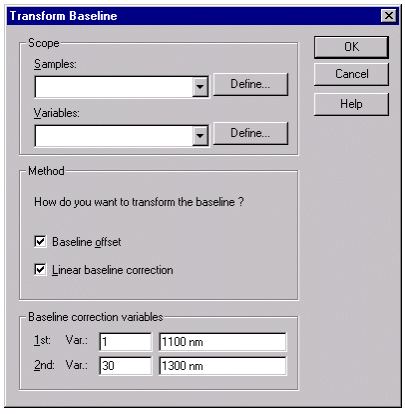
Finally, enter the Polynomial order, i.e. the order of the polynomial to be fitted. A polynomial order of 2 means that a second-degree equation will be used to fit the data points. A higher number means a more flexible polynomial, i.e. a more precise differentiation.

Note that, after the operation is completed, the data will be slightly truncated at both ends. If *p* is the number of left side points and *q* the number of right side points in the smoothing segment, the first *p* and the last *q* variables in the smoothed variable set will be set to zero. This is because there are not enough points to the left (resp. right) of these variables to compute the smoothing function.

Modify - Transform - Baseline

Baseline offset and **Linear baseline correction** are transformations used to correct the baseline of samples, and are set in the dialog **Transform Baseline**. They are mostly used for spectroscopic purposes. The two transformations can be executed separately or together, in the combined case the Linear baseline correction will be run first, then the Baseline offset.

Dialog: Transform Baseline



First select the Sample and Variable sets that define the matrix you want to correct in the **Scope** field. Then select the wanted transformation. If you select **Linear Baseline Correction** you have to select the two variables which define the new baseline. The first and last variable are selected by default. The Define buttons in the **Scope** field take you to the **Set Editor** where you can define new sample and/or variable sets.

Baseline Offset

The formula for the baseline offset correction can be written as follows:
f(x) = x – min(X),
where x is a variable and X denotes all selected variables for this sample

For each sample, the value of the lowest point in the spectrum is subtracted from all the variables. The result of this is that the minimum value is set as 0 and the rest are positive values. To use this consistently for a set of samples, make sure that the lowest point pertains to the same variable for all samples.

Linear Baseline Correction

This transformation transforms a sloped baseline into a horizontal baseline. The technique is to point out two variables which should define the new baseline. These are both defined as 0, and the rest of the variables are transformed according to this with linear interpolation/extrapolation. You should take precautions not to select as basis variables that have spectroscopic bands. As for the offset correction, make sure that the lowest points pertain to the same variables for all samples.

Modify - Transform - SNV

Standard Normal Variate (SNV) is a row-oriented transformation which removes scatter effects from spectra by centering and scaling each individual spectrum.

Each value in a row of data is transformed according to the formula:
New value = (Old value – mean (Old row)) / Stdev (Old row)

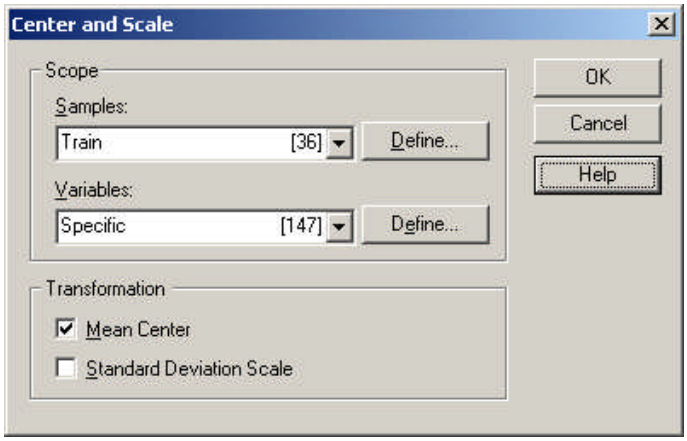
In the dialog **Standard Normal Variate**, select the Sample and Variable sets that define the matrix you want to correct in the **Scope** field. The Define buttons take you to the **Set Editor** where you can define new sample and/or variable sets.

Modify - Transform - Center and Scale

Centering and/or scaling your data may be useful to study the data in various plots from the Plot menu in the Editor, or prior to running **Task - Statistics**. It may for example allow you to compare the distributions of variables of different scales within one plot.

These two transformations are column-oriented: the transformed values are computed as a function of the values in the same column of the table.

Dialog: Center and Scale



In the dialog **Center and Scale**, select the Sample and Variable sets that define the matrix you want to correct in the **Scope** field. The Define buttons take you to the **Set Editor** where you can define new sample and/or variable sets.

In the **Transformation** frame, two options are available:

- Mean Center – within the selected sample and variable scope, it subtracts the mean of all samples in the column (i.e. variable mean) from each cell of the column.
- Standard Deviation Scale – within the selected sample and variable scope, it divides each cell of the column by the standard deviation of the column (i.e. variable Sdev).

Each option can be selected either separately or together with the other.

Note 1: If you only want to display the mean and standard deviation of the variables in your table, use menu option **View - Variable Statistics**.

Note 2: The Center and Scale transformations are *not* supported in auto-pretreatments. See next note.

Note 3: The PCA and Regression dialog boxes include options for centering and scaling variables directly at the analysis stage. It is **recommended to perform centering and scaling at the model-building stage**, in case you need the model for future prediction or classification. The same centering and scaling options will be applied as when the model was built.

Note 4: Centering and/or scaling the data more than once will not affect the structure of the data any further. Consequently, if you have applied a Center and Scale transformation to your data from the Editor, the data may harmlessly be re-centered and/or re-scaled at the modeling stage (PCA or regression).

Modify - Transform - Reduce (Average)

You can reduce the size of your data table by averaging samples or variables. Averaging reduces uncertainty in the measurements and the effect of noise. If you have the same number of replicates in your data table, you can average the replicates to get one row for each sample. Depending on whether you reduce along samples or variables, the transformation is either column-oriented or row-oriented.

Choose whether to Reduce along Variables or Samples in this field in the **Reduce (Average)** dialog. The number of adjacent samples or variables to be averaged must be given in the Reduction Factor field.

Note: All defined sets will be adjusted according to the reduction you perform.

Reduce (Average) 3-D Data

Reducing by averaging is disabled because it would change the dimensions of the data table.

Useful tips

1- Depending on your applications, it may be relevant to average your data over all Secondary variables for an OV^2 layout (resp. samples for an O^2V layout). To do so, select the whole table then drag and drop it unto an empty spot of the workspace (alternatively use **File - Duplicate - As 2-D Data Table**). The resulting 2-D table can be averaged any way you wish.

If you reduce your data so that all Secondary variables are collapsed into an average for each Primary variable, then you are left with Primary variables only and it is quite logical that the result should be stored as 2-D data table.

2- You may use a similar trick to average in a flexible way over the samples (OV^2 layout) or variables (O^2V layout) of your 3-D table. The rows (resp. columns) containing the averaged values can then be copied back to your original 3-D data table.

Modify - Transform - Transpose

This command transposes the complete data table. Designed data tables cannot be transposed. Category variables are automatically split when you transpose a table containing such variables.

Note: All defined sets are also transposed.

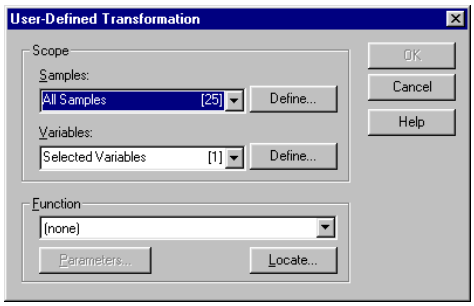
Transpose (3-D)

Transpose is disabled because it would change the dimensions of the data table. Swapping the 3-D layout may be more relevant than a standard transposition. Try it with **Modify - Swap 3-D Layout**, **Modify - Toggle 3-D Layouts** or **Modify - Swap Samples & Variables**.

Modify - Transform - User-defined

This function lets you select your own (user-defined) transformation that you can apply on a selection of samples and variables. These transformation components can be developed separately, and installed on the computer when needed. A wide range of modifications can be done by such components, including deleting and inserting both variables and samples.

Dialog: User-Defined Transformation

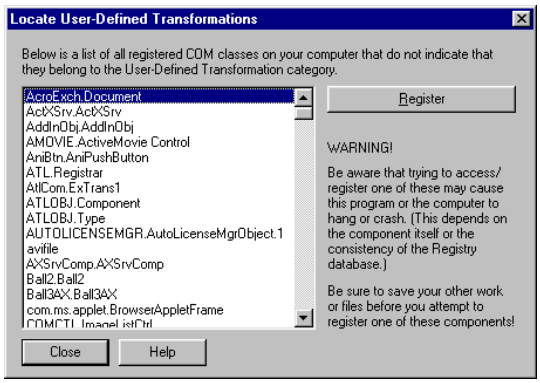


In the Scope field in the **User-Defined Transformation** dialog, select the sample and variable sets that define the matrix you want to modify. If necessary, select Define to enter the **Set Editor** and define new sets. Then select a function of an installed UDT component in the Function drop-down menu. If a valid function is selected, the OK button is enabled, and you can click it to complete the transformation.

Some UDT components may allow additional parameters to be configured (possibly depending on the current size of your selected scope). Whenever such a configuration is available for the selected function, the Parameters button is enabled. By selecting it, a function-specific dialog box will appear, allowing you to set various parameters. Note, however, that the default parameters will be re-selected every time you make a selection from the Function drop-down menu.

If your function is not listed, but probably installed on the computer, you can try to locate and register it by selecting Locate. The **Locate User-Defined Transformations** dialog will be shown.

Dialog: Locate User-Defined Transformations


Locate User-Defined Transformations
Below is a list of all registered COM classes on your computer that do not indicate that they belong to the User-Defined Transformation category.
AcroExch.Document
ActXSrv.ActXSrv
AddInObj.AddInObj
AMOVIE.ActiveMovie Control
AniBtn.AniPushButton
ATL.Registrar
AtlCom.ExTrans1
ATLOBJ.Component
ATLOBJ.Type
AUTOLICENSEMGR.AutoLicenseMgrObject.1
avifile
AXSrvComp.AXSrvComp
Ball2.Ball2
Ball3AX.Ball3AX
com.ms.applet.BrowserAppletFrame
Register
WARNING!
Be aware that trying to access/ register one of these may cause this program or the computer to hang or crash. (This depends on the component itself or the consistency of the Registry database.)
Be sure to save your other work or files before you attempt to register one of these components!
Close
Help

If the UDT component is properly installed, you will now find it on the list shown (along with many other non-UDT components installed). Select the component in the list, and click Register to let The Unscrambler try to register and access it as a UDT component. A short information message will be displayed to tell you whether the registration attempt succeeded or failed. Select Close to return to the **User-Defined Transformation** dialog.

Warning!

Trying to register a component may potentially cause The Unscrambler or your computer to hang or crash. This is beyond the control of The Unscrambler, and most likely due to the component itself or because of an inconsistency in the underlying Registry database. You should make sure you have saved your other work before attempting to register, so you do not run the risk of losing important data in case of a crash.

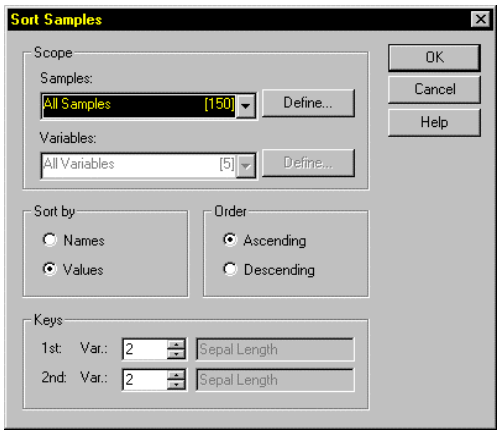
User-defined (3-D)

User-defined transformations are disabled on 3-D data.

Modify - Sort Samples…

With the help of this option you can sort your samples by the names or values in one or two variables. You cannot sort samples with locked cells (e.g. designed data). All defined sets are kept during the sorting.

Dialog: Sort Samples



You define how you want to sort the samples in the **Sort Samples** dialog. First, select the sample and variable sets that you want to sort in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets.

In the Sort by field, you select whether you want to sort the samples by their names or the values of given variables, and in the field Order whether the samples are to be sorted with the highest values at the top (descending) or the lowest value at the top (ascending).

The Keys field is only enabled if you have chosen to sort by values. Here, you must specify the variable to use as 1st and 2nd key. The samples will first be sorted by the first key, then by the second key.

Modify - Sort Samples (3-D)

Sorting is disabled in 3-D tables with an O^2V layout, since this would disturb the Primary / Secondary structure of the samples.

Modify - Sort Samples by Sets

When using this option, all samples belonging to Sample Set #1 are displayed in the first rows of the data table, followed by samples from Sample Set #2, etc… The sorting order is defined by the alphabetic order in which the Sets are displayed as a list in the **Set Editor**.

Samples that do not belong to any set are displayed at the end of the table.

If the sample sets currently defined in your data table are overlapping, the command opens the **Select Sample Sets To Sort** dialog, where you can choose which sets must be taken into account for the sorting operation.

Note1: This option is only available when at least one Sample Set is defined.

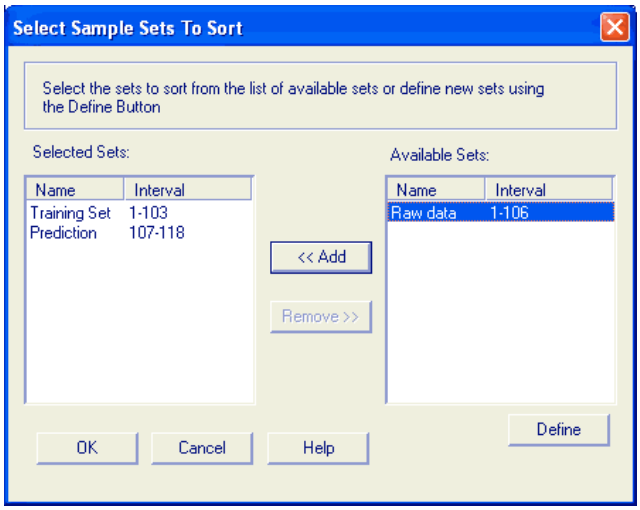
Note2: You cannot sort samples with locked cells (e.g. designed data).

Undo / Redo **Modify - Sort Samples by Sets** with the corresponding options of the **Modify** menu.

Select Sample Sets To Sort / Select Variable Sets To Sort Dialog

This dialog has the same shape for sorting ***Samples*** or ***Variables*** by sets.

Dialog: Select Sample Sets To Sort



Sort Samples by Sets

Select the sample set that must be placed in the first rows of your data table from the list of Available Sets, and click on the Add button. The chosen set is moved to the list of Selected Sets. Proceed similarly to select the second sample set, which will be placed in the following rows of the table, then the third sample set, etc.

Note: After sorting, samples that do not belong to any selected set will be displayed at the end of the table.

Sort Variables by Sets

Select the variable set that must be placed in the first columns of your data table from the list of Available Sets, and click on the Add button. The chosen set is moved to the list of Selected Sets. Proceed similarly to select the second variable set, which will be placed in the following columns of the table, then the third variable set, etc.

Note: After sorting, variables that do not belong to any selected set will be displayed at the end of the table.

Common Features

Overlapping sets cannot be placed simultaneously in the list of Selected Sets.

Click Define if you need to define new sets; this will lead you to the **Set Editor** dialog.

Modify - Sort Variables by Sets

When using this option, all variables belonging to Variable Set #1 are displayed in the first rows of the data table, followed by variables from Variable Set #2, etc… The sorting order is defined by the alphabetic order in which the Sets are displayed as a list in the **Set Editor**.

Variables that do not belong to any set are displayed at the end of the table.

If the variable sets currently defined in your data table are overlapping, the command opens the **Select Variable Sets To Sort** dialog, where you can choose which sets must be taken into account for the sorting operation.

Note1: This option is only available when at least one Variable Set is defined.

Note2: You cannot sort variables with locked cells (e.g. designed data).

Modify - Sort Variables by Sets can be undone / redone with the corresponding options of the **Modify** menu.

Modify - Sort Variables by Sets (3-D)

Sorting is disabled in 3-D tables with an OV^2 layout, since this would disturb the Primary / Secondary structure of the variables.

Modify - Shift Variables…

You can shift variables up or down in the data table. This is often used for time-related measurements, e.g. process data. Shifting variables will generate time lags between the various measurements. It is a column-oriented transformation, i.e. the contents of a cell are likely to be influenced by its vertical neighbors.

In the **Shift Variables** dialog, choose the appropriate variable set in the Scope field. If necessary, press Define to enter the **Set Editor** and define new sets.

Use the radio buttons in the Direction field to decide whether the defined set of variables is to be shifted up or down. Specify by how many rows the variables should be moved in the Units field.

Note: All rows of the table are affected by this operation.

The new cells created by this action are filled with “m” (“missing values”) as illustrated below:

Shifting variables creates new cells in the data table

Before Variable Shift

A	**B**	**C**
0.25	0.54	1.64
0.13	1.24	3.01
1.11	1.82	0.14
0.24	0.25	1.12
0.79	1.45	0.91
1.45	3.21	0.42

…

After shifting variable C down 1

A	**B**	**C**
0.25	0.54	**m**
0.13	1.24	1.64
1.11	1.82	3.01
0.24	0.25	0.14
0.79	1.45	1.12
1.45	3.21	0.91
m	**m**	0.42

Modify - Shift Variables (3-D)

Shifting variables is disabled for 3-D data tables because it would change the dimensions of the data table.

Modify - Reverse Sample Order

This option reverses the order of samples in your data table from last to first.

All Sample Sets are automatically updated accordingly, as with any other sorting option.

Note: Using this option, sorting is always performed on the whole data table.

Modify - Reverse Sample Order (3-D)

This option is disabled in 3-D tables with an O^2V layout, since this would disturb the Primary / Secondary structure of the samples.

Modify - Reverse Variable Order

This option reverses the order of variables in your data table from last to first.

All Variable Sets are automatically updated accordingly, as with any other sorting option.

Note: Using this option, sorting is always performed on the whole data table.

Modify - Reverse Variable Order (3-D)

This option is disabled in 3-D tables with an OV^2 layout, since this would disturb the Primary / Secondary structure of the variables.

Modify - Swap 3-D Layout

Choose **Modify - Swap 3-D Layout** to re-format a 3-D table from OV^2 to O^2V or vice-versa.

From OV^2 to O^2V, secondary variables become secondary samples. From O^2V to OV^2, secondary samples become secondary variables. Sample / variable names are also updated. Primary variables and primary samples remain unchanged in either case.

The operation can be undone using **Modify - Undo Swap 3-D Layout** or CTRL-Z.

Modify - Swap Samples & Variables

Choose **Modify - Swap Samples & Variables** to change the layout of a 3-D table in a flexible way.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Here are all the choices to be found under the **Modify - Swap Samples & Variables** menu option:

Modify - Swap Samples & Variables - Pri Variable & Sec Variable

Modify - Swap Samples & Variables - Pri Variable & Sample

Modify - Swap Samples & Variables - Sec Variable & Sample

Modify - Swap Samples & Variables - Pri Sample & Sec Sample

Modify - Swap Samples & Variables - Pri Sample & Variable

Modify - Swap Samples & Variables - Sec Sample & Variable

Modify - Swap Samples & Variables - Pri Variable & Sec Variable

Use this option to exchange Primary variables and Secondary variables in a 3-D table with layout OV^2.

As a result:

- Former Primary variables are now Secondary variables;
- Former Secondary variables are now Primary variables;
- Variable names are updated accordingly;
- Former Samples are still Samples.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Swap Samples & Variables - Pri Variable & Sample

Use this option to exchange Primary variables and Samples in a 3-D table with layout OV^2.

As a result:

- Former Primary variables are now Samples;
- Former Samples are now Primary variables;
- Variable names and Sample names are updated accordingly;
- Former Secondary variables are still Secondary variables.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Swap Samples & Variables - Sec Variable & Sample

Use this option to exchange Secondary variables and Samples in a 3-D table with layout OV^2.

As a result:

- Former Secondary variables are now Samples;
- Former Samples are now Secondary variables;
- Variable names and Sample names are updated accordingly;
- Former Primary variables are still Primary variables.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Swap Samples & Variables - Pri Sample & Sec Sample

Use this option to exchange Primary samples and Secondary samples in a 3-D table with layout O^2V.

As a result:

- Former Primary samples are now Secondary samples;
- Former Secondary samples are now Primary samples;
- Sample names are updated accordingly;
- Former Variables are still Variables.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Swap Samples & Variables - Pri Sample & Variable

Use this option to exchange Primary samples and Variables in a 3-D table with layout O^2V.

As a result:

- Former Primary samples are now Variables;
- Former Variables are now Primary samples;
- Variable names and Sample names are updated accordingly;
- Former Secondary samples are still Secondary samples.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Swap Samples & Variables - Sec Sample & Variable

Use this option to exchange Secondary samples and Variables in a 3-D table with layout O^2V.

As a result:

- Former Secondary samples are now Variables;
- Former Variables are now Secondary samples;
- Variable names and Sample names are updated accordingly;
- Former Primary samples are still Primary samples.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Modify - Toggle 3-D Layouts

Choose **Modify - Toggle 3-D Layouts** or CTRL-3 for a quick change of the layout of a 3-D table.

This is a quick way to perform the 2x6 operations otherwise available under **Modify - Swap 3-D Layout** and **Modify - Swap Samples & Variables**.

By using CTRL-3 repeatedly you will achieve the following results:

Result of toggling 3-D layouts repeated times on an OV^2 or O^2V table

Layout after …	# times CTRL-3	Layout after …	# times CTRL-3
OV^2 (s , pv * sv)	0	O^2V (ps * ss , v)	0
OV^2 (s , sv * pv)	1	O^2V (ss * ps , v)	1
OV^2 (sv , s * pv)	2	O^2V (v * ps , ss)	2
OV^2 (pv , s * sv)	3	O^2V (v * ss , ps)	3
OV^2 (pv , sv * s)	4	O^2V (ss * v , ps)	4
OV^2 (sv , pv * s)	5	O^2V (ps * v , ss)	5
O^2V (sv * s , pv)	6	OV^2 (ps , ss * v)	6
O^2V (s * sv , pv)	7	OV^2 (ps , v * ss)	7
O^2V (pv * sv , s)	8	OV^2 (v , ps * ss)	8
O^2V (pv * s , sv)	9	OV^2 (ss , ps * v)	9
O^2V (s * pv , sv)	10	OV^2 (ss , v * ps)	10
O^2V (sv * pv , s)	11	OV^2 (v , ss * ps)	11

Note: Although all combinations are exhausted after 12 times, you need to apply CTRL-3 16 times if you want to get back to the original layout.

The operation can be undone using **Modify - Undo Swap Sams & Vars** or CTRL-Z.

Note: Only the last operation can be undone! If you have already applied CTRL-3 several times, continue until you get back to the original layout.

Modify - Undo

or **Ctrl+Z**

This option reverses the last operation you performed on your data in the Editor. The following operations can be undone:

From the Edit menu:

- Cut;
- Paste;
- Fill;
- Insert;

- Append;
- Delete;
- Convert to Category variable;
- Correct Mixture Components;
- Convert to Mixture Variables.

From the Modify menu:

- Compute;
- Transform;
- Sort Samples;
- Sort Samples by Sets;
- Sort Variables by Sets;
- Shift Variables;
- Reverse Sample order;
- Reverse Variable order;
- Swap 3-D Layout;
- Swap Samples & Variables;
- Toggle 3-D Layouts.

An undone operation can be re-done with **Modify - Redo**.

Note1: You can only undo an editing operation if it is the most recent operation you have performed.

Note2: To access the **Undo** and **Redo** buttons, activate the **Main Editor Toolbar** (use menu **View - Toolbars…** from the Editor)

Modify - Redo

or **Ctrl+Y**

You can recover the results of an editing operation you have just undone (see chapter Modify - Undo) with the help of the **Redo** command.

The following operations can be re-done:

From the Edit menu:

- Cut;
- Paste;
- Fill;
- Insert;
- Append;
- Delete;

- Convert to Category variable;
- Correct Mixture Components;
- Convert to Mixture Variables.

From the Modify menu:

- Compute;
- Transform;
- Sort Samples;
- Sort Samples by Sets;
- Sort Variables by Sets;
- Shift Variables;
- Reverse Sample order;
- Reverse Variable order;
- Swap 3-D Layout;
- Swap Samples & Variables;
- Toggle 3-D Layouts.

Modify - Properties

This command launches the **Properties** dialog, where the properties of a sample or variable can be viewed and - in some cases - modified. The command is also available by right-clicking on a sample or variable number.

Select the sample or variable for which you wish to view the properties. This will launch one of the following dialogs:

Sample X - Properties

In this dialog you can change the name of the active sample in the Name field. You can also see what kind of sample it is in the Type field. All samples in non-designed data tables are defined as normal. Samples in designed data tables can be of the types listed below:

Sample types in designed data tables

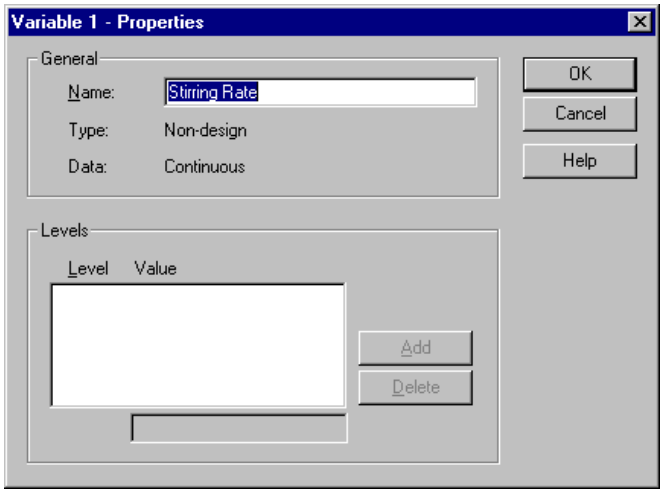
Sample Type	Description
Normal	A sample with a normal combination of variable levels.
Cube	A sample with a combination of high and low levels in a design.
Center	A sample with mean values for all variables.
Star	A sample used in Central Composite Designs, with extreme values of one design variable and average values of the others.
Vertex	A sample used in Mixture or D-optimal designs, located at a “corner”.
Centroid	A sample used in Mixture or D-optimal designs, located at the center of an edge or face.

Interior	A sample used in Mixture designs, located inside the simplex.
Reference	A sample with response data only. The design variables have missing data.

Variable X - Properties

In the General field in the **Variable Properties** dialog you can modify the name of the active variable in the Name field and see whether it is a design variable or a non-design variable in the Type field. The Data field displays the data type - category or continuous.

Dialog: Variable Properties



The field Levels displays the levels of the chosen variable. The number of levels in designed data tables is fixed and cannot be changed. Hence, the Add and Delete buttons will be disabled. You can however change the levels of the variable by selecting the level you wish to change and typing in the new value in the field below the list. Click once in the list to update it.

Note: Do not change the levels of continuous variables unless you have a very good reason to do it.

For category variables, you change the values of the levels in the same way as for continuous variables. In addition, you may Add or Delete levels. Delete will remove the selected level, and pressing Add will add a new level, allowing you to enter the value in the field below the list. Click once in the list to update it.

If you have selected more than one variable in the Editor, the properties of the first variable are shown. In such a multi-selection, you can only change the variable name, not the levels.

Modify - Layout…

or **Ctrl+L**

Through this option you can change the layout of the data values of selected variables in the **Layout** dialog. The layout settings only affect the visual representation of the data.

Select the default format of the data values in the Numeric format field. The three possibilities are displayed below. Use the spin button to select the number of decimal places to display in the data table. Values stored with more decimal places are rounded to the number you select.

Numeric format options

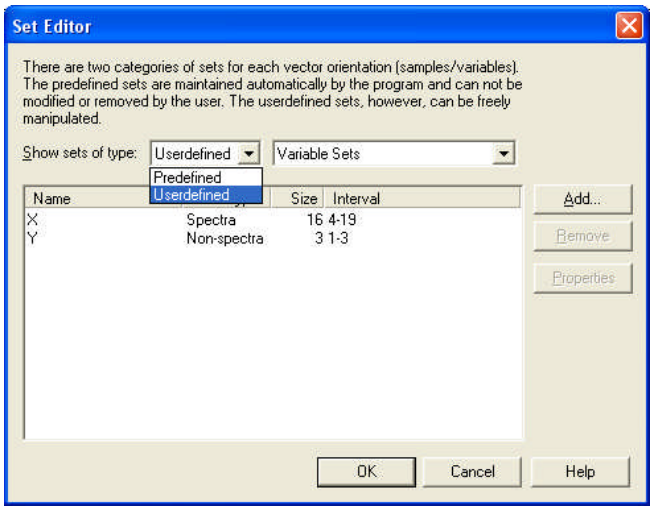
Option	Description
Autofit	The Unscrambler decides the format
“12345.6789”	Normal layout
“1.2345e+04”	Scientific notation

Note: This operation applies to the selected variables only. If you wish to change the default layout of all variables in all tables, you can use the System Setup dialog.

Modify - Edit Set…

In the **Set Editor** dialog, you can define sets to be used for data selection, plotting, transformation and analysis. A set is a vital part of the philosophy behind handling data with The Unscrambler.

Dialog: Set Editor



The very first thing you need to do in the Set Editor is to select whether you want to specify a new Sample or Variable Set. This is done from the drop-down list in the field Show sets of type.

Note: Always make sure that you are displaying the correct set type, i.e. that you have made the correct choice in the “Show sets of type” field.

Depending on your choice of set type, i.e. Sample or Variable Sets, the list below will display all current sets defined by you or any other User. You can delete an already defined set by selecting it on the list and pressing Remove.

In addition, The Unscrambler automatically predefines certain sets, such as All Samples and All Variables. These cannot be altered, but you may view their contents by selecting “Predefined” from the Show sets of type field.

Define new sets by pressing the Add… button. This will launch the **New Sample Set/New Variable Set** dialog respectively.

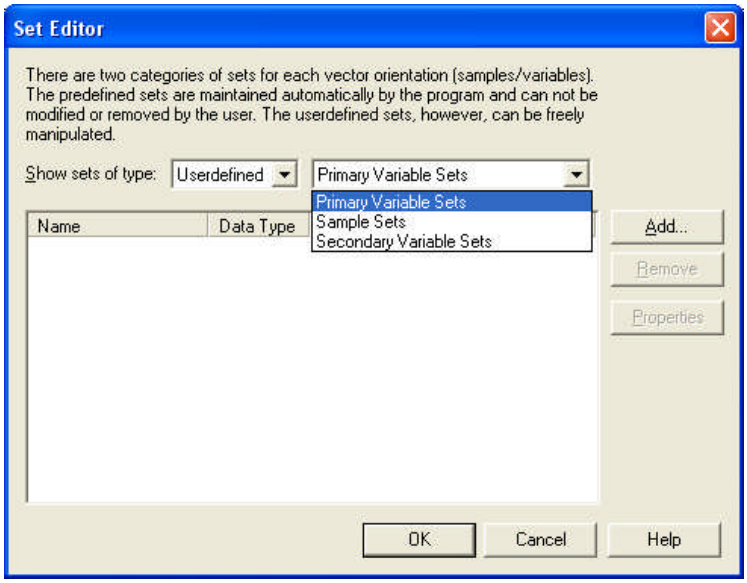
If you select an existing set and press the Properties button, you can change the set definition in the **Modify Sample Set/Modify Variable Set** dialog. This is identical to the **New … Set** dialog.

Modify - Edit Set: 3-D data table

Since 3-D data tables have an extra dimension, the **Set Editor** dialog allows you to edit three types of user-defined sets instead of two.

For an OV^2 table, these are: Primary Variable Sets, Sample Sets and Secondary Variable Sets, as shown below.

Dialog: Set Editor (3-D data table)


Set Editor
There are two categories of sets for each vector orientation (samples/variables). The predefined sets are maintained automatically by the program and can not be modified or removed by the user. The userdefined sets, however, can be freely manipulated.
Show sets of type:
Userdefined
Primary Variable Sets
Primary Variable Sets
Sample Sets
Secondary Variable Sets
Name
Data Type
Add...
Remove
Properties
OK
Cancel
Help

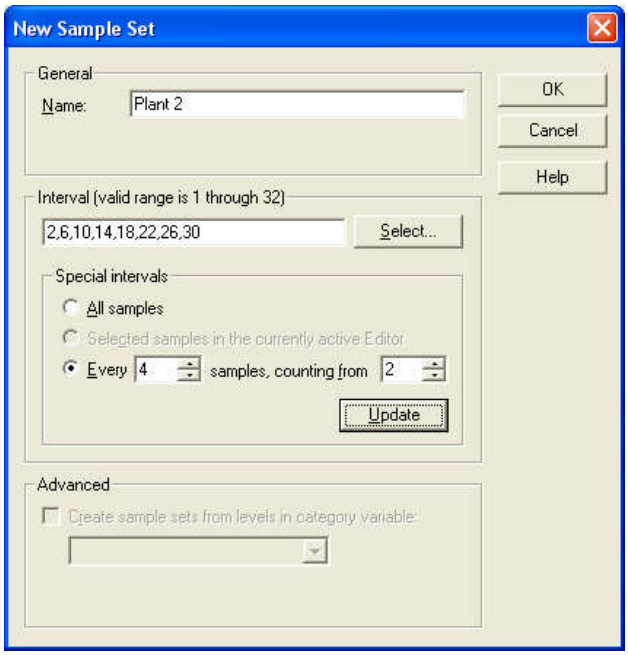
Note: Since no analysis is allowed on a 3-D table with layout O^2V, the Set Editor is disabled for such tables.

New Sample Set Dialog

Allows you to specify a new sample set (or modify its properties).

In the **General** section, give the new set a name in the Name field. This is the name that will refer to the set in other dialogs when you want to make models, plot data, etc. It should therefore be evocative of the nature of the samples in the set.

Dialog: New Sample Set



In the **Interval** section, enter the sample range. Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27. Pressing the Select button next to this field launches an Editor (the **Select Samples** dialog) which allows you to select samples by clicking on them.

In the Special intervals field you can enter the set interval by using the currently selected samples in the Editor. Every *n*th sample can also be entered into the set. Specify the value of n with the spin buttons. To enter the special set intervals into the Set Interval box, press Update.

The **Advanced** field at the bottom allows you to select a Category Variable from a drop-down list and automatically create one new Sample Set for each level of the Category Variable.

Note: Samples with missing value of the Category Variable will not be included into any of the new Sample Sets.

New Variable Set Dialog

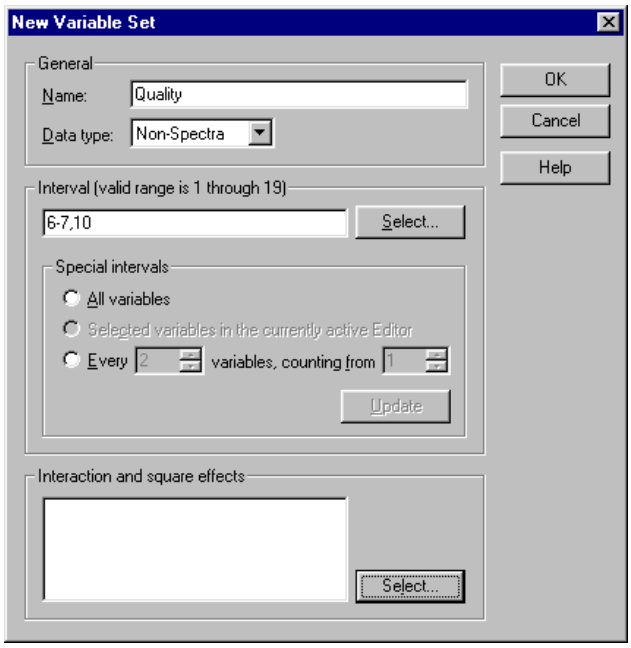
Allows you to specify a new variable set (or modify its properties).

In the **General** section, give the new set a name in the Name field. This is the name that will refer to the set in other dialogs when you want to make models, plot data, etc. It should therefore be evocative of the nature of the variables in the set.

Variable Sets may be of type **Spectra** or **Non-spectra**. Results from models where sets marked as Spectra are used have different default plots. For instance, the loadings are plotted as line plots instead of 2D Scatter plots.

Make your choice between Spectra or Non-spectra in the Data type field.

Dialog: New Variable Set



In the **Interval** section, enter the variable range. Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27. Pressing the Select button next to this field launches an Editor (the **Select Variables** dialog) which allows you to select variables by clicking on them.

In the Special intervals field you can enter the set interval by using the currently selected variables in the Editor. Every *n*th variable can also be entered into the set. Specify the value of n with the spin buttons. To enter the special set intervals into the Set Interval box, press Update.

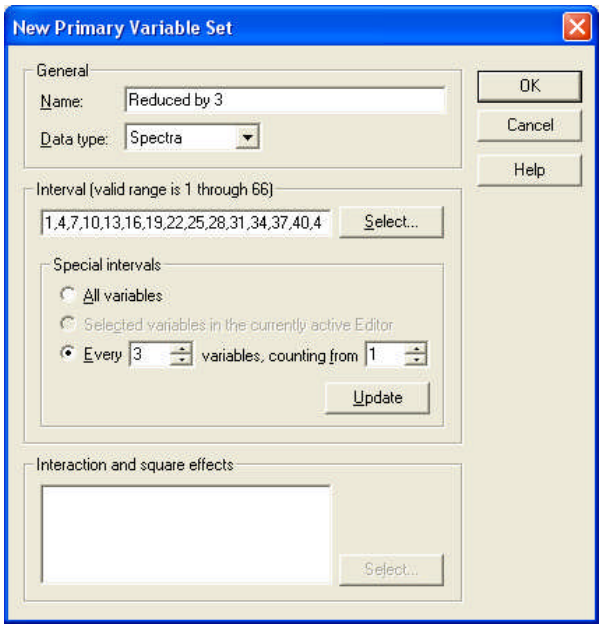
Finally, you have the possibility to include Interaction and square effects in your new set in this field. Press Select to launch the **Interaction and Square Effects Selection** dialog.

Note: You can only include interaction and square effects in sets which include design variables.

New Primary Variable Set Dialog

Allows you to specify a new Primary Variable set (or modify its properties).

Dialog: New Primary Variable Set



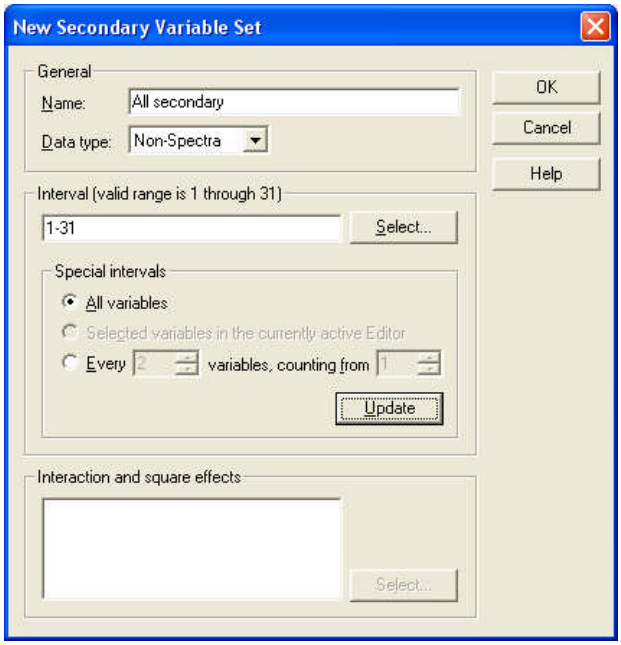
This dialog operates in the same way as the **New Variable Set** dialog (see p.246).

Note: Interaction and square effects are disabled in Primary Variable sets.

New Secondary Variable Set Dialog

Allows you to specify a new Secondary Variable set (or modify its properties).

Dialog: New Secondary Variable Set



This dialog operates in the same way as the **New Variable Set** dialog (see p.246).

Note: Interaction and square effects are disabled in Secondary Variable sets.

Modify Sample Set Dialog

Allows you to modify the properties of an existing Sample Set.

Lookup the detailed dialog description in New Sample Set Dialog p.245.

Modify Variable Set Dialog

Allows you to modify the properties of an existing Variable Set.

Lookup the detailed dialog description in New Variable Set Dialog p.246.

Modify Primary Variable Set Dialog

Allows you to modify the properties of an existing Primary Variable Set.

Lookup the detailed dialog description in New Primary Variable Set Dialog p.247.

Modify Secondary Variable Set Dialog

Allows you to modify the properties of an existing Secondary Variable Set.

Lookup the detailed dialog description in New Secondary Variable Set Dialog p.248.

New Sample Set/Modify Sample Set and New Variable Set/Modify Variable Set

When you press Add in the **Set Editor** you enter the **New Sample Set** or **New Variable Set** dialog. The two dialogs are quite similar.

When you press Properties in the **Set Editor** you enter the **Modify Sample Set** or **Modify Variable Set** dialog. These two dialogs are identical to **New Sample Set** and **New Variable Set** respectively.

Note: If you are editing a 3-D data table, you may also enter one of the following dialogs: **New Primary Sample Set**, **New Secondary Sample Set**, **New Primary Variable Set**, **New Secondary Variable Set**, **Modify Primary Sample Set**, **Modify Secondary Sample Set**, **Modify Primary Variable Set**, **Modify Secondary Variable Set**. These dialogs are all identical to **New Sample Set** and **New Variable Set** respectively.

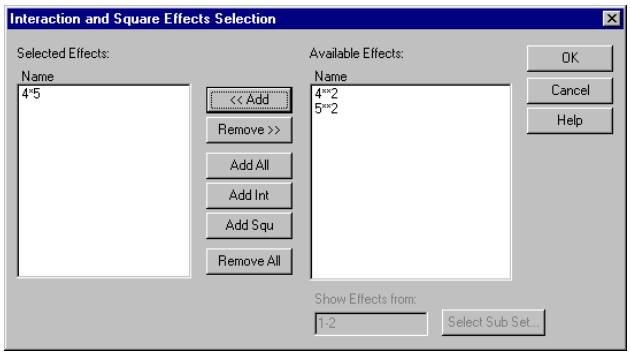
For more details on the fields available in each dialog, lookup the one you are interested in hereafter:

- New Sample Set Dialog p.245
- New Variable Set Dialog p.246

Interaction and Square Effects Selection Dialog

When you press the Select button to the right of the Interaction and square effects field in the **New Variable Set** dialog, you enter the **Interaction and Square Effects Selection** dialog, where you can specify combinations of variables (cross-products of two variables, also called Interactions, or squares of individual variables) to be taken into account in your model.

Dialog: Interaction and Square Effects Selection



The dialog contains two lists; Selected Effects to the left and Available Effects to the right. The latter lists all available effects with their full names.

Select the combinations you wish to include and press the Add button to include them in the leftmost list under short names.

You can also Add All, Add Int (i.e. Interaction Effects) and Add Squ (i.e. Square Effects).

Use the Remove or Remove All buttons to remove effects from the leftmost list.

Note: If your Variable Set contains more than 62 variables, you must push the Select sub-set button to define a set with max. 62 variables before you can select effects.

The maximum number of interactions that can be added is 1891.

Select Samples / Select Variables Dialog

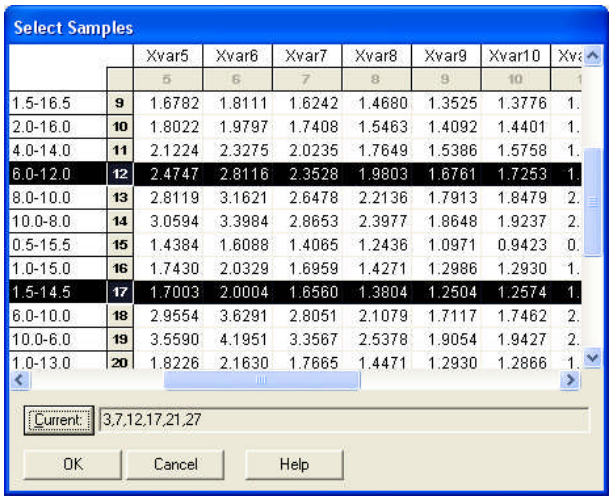
This dialog allows you to select samples or variables directly from a data table. It is accessed by clicking the Select button in another dialog. Typical situations are:

- From the **New Sample Set** or **Modify Sample Set** dialog: selecting samples to be included in a Sample Set
- From the **New Variable Set** or **Modify Variable Set** dialog: selecting variables to be included in a Variable Set
- From the Samples sheet of any Task dialog (e.g. **Statistics**, **PCA** etc.): selecting samples to be kept out from the analysis
- From the Variables sheet of any Task dialog (e.g. **Statistics**, **PCA** etc.): selecting variables to be kept out from the analysis

The dialog consists of a small Editor window that displays the relevant portion of your data table (for instance, the active sample set and variable set for a PCA) and a few buttons.

The **Select Samples** dialog is described in detail hereafter. The description can easily be applied to the **Select Variables** dialog by replacing “sample” with “variable” and “row” with “column”.

Dialog: Select Samples



Click on the ***grey*** cell displaying Sample Number (e.g. 12) to select one sample.

Include several Sample Numbers in one click if you want to perform a continuous selection.

Alternatively, click on the first Sample Number you want (e.g. 3), then scroll down, press ***<Shift> and click*** on the last one (e.g. 15) you want to include in your selection, to achieve a ***continuous*** selection (e.g. 3-15).

Use ***<Ctrl> + click*** to select several samples in a ***non-continuous*** range (e.g. 12, 17).

Note: In some cases, multiple selection may be disabled. Example: selecting a Reference Spectrum as Background Information for EMSC – the dialog does not allow for more than ***one*** sample in the selection.

You may ***scroll*** up/down and right/left whenever necessary.

At any time, you may ***check your current selection*** by clicking Current; the selected sample numbers will be displayed in the field next to that button (e.g. 3,7,12,17,21,27).

When you are satisfied with your selection, click OK to go back to the previous dialog; else click Cancel.

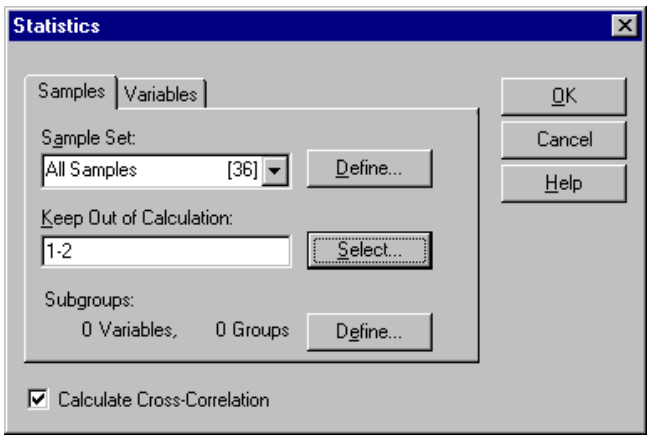
The Task Menu

Task - Statistics…

This dialog is used to compute the means, standard deviations, correlations and percentiles of measurements.

You specify the samples and variables you want to work with in the **Statistics** dialog, which contains 2 sheets; Samples and Variables, as well as one general option. You can also group samples according to levels of the variables in the data table.

Dialog: Statistics



General Options

The box Calculate Cross-Correlation is available regardless of which sheet you are on. Tick this box if you want to calculate the cross correlation between the variables. Once the statistics have been computed, you may save the result file and later import the cross-correlation matrix StatCorr using **File - Import - Unscrambler Results.**

Note: Computing cross-correlations may be time and memory consuming; turn off this option if you do not need the results.

Statistics Dialog: Samples Sheet

Choose the Sample Set on which you want to base the calculations from the Sample Set drop-down list. Statistics are calculated for the entire chosen sample set. If you want to define a new set, click Define to launch the **Set Editor** dialog.

If you want to exclude some of the samples from the analysis, type in their numbers in the field Keep Out of Calculation, or click Select to choose them directly from an Editor (the **Select Samples** dialog). Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27.

Note** - How to use **Sample Set** and **Keep Out:

- In Sample Set you select the general sample "population" the analysis applies to.
- In Keep Out… you remove one (or more) of these samples if it turns out that they disturb the results.

The computations will always be performed on a default group of samples containing all the samples you have included in the analysis. This group is called “All samples”.

In addition, they can also be performed on smaller groups of samples determined by the levels of one or more of the variables in your data table. The variables which have the ability to ***generate groups*** of samples are ***leveled*** variables (category variables and design variables).

For instance, if you are computing statistics for variable “Quality”, and your data table contains a category variable called “Equipment” with two levels “New” and “Old”, your statistics result file will contain Quality statistics for the following groups of samples:

1- All samples;

2- Samples which come from the New Equipment;

3- Samples which come from the Old Equipment.

Note: If you have category variables or design variables in your table, each level of each of these variables will automatically define a group. No need to include those leveled variables in the analysis!

For a ***designed data table***, more groups are automatically defined: Design samples, Center samples, Reference samples, whenever relevant.

If there are ***more than two leveled variables*** in the data table, you have the additional possibility of defining ***subgroups*** based on ***combinations*** of the levels of at least two of those variables. In the Subgroups field, click Define to choose the leveled variables you want to use.

For instance, if you choose variables “Equipment” (2 levels: “New”, “Old”) and “Week” (3 levels: “36”, “37”, “38”), you will get statistics for each of the 6 subgroups “New equipment * Week 36”, “Old Equipment * Week 36”, etc., in addition to all pre-existing groups (All samples, New equipment, Old equipment, Week 36, etc.).

Statistics Dialog: Variables Sheet

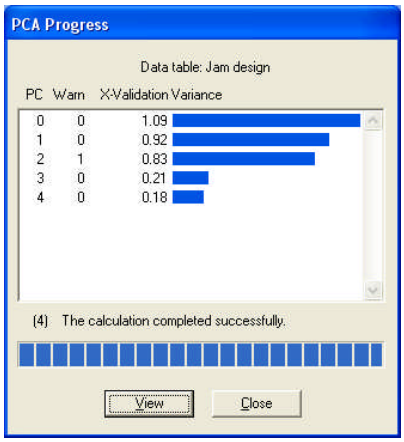
On the Variables sheet you decide on which Variable Set to perform the statistical calculations in the Variable Set field. Only continuous variables may be chosen. If there are any category variables in your selection, they will be automatically excluded from the analysis. To define new variable sets, click Define to go to the **Set Editor**.

If you want to exclude some of the variables from the analysis, type in their numbers in the field Keep Out of Calculation, or click Select to choose them directly from an Editor Editor (the **Select Variables** dialog). Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27.

Progress Dialog

This dialog pops up after you have clicked OK in a Task dialog (e.g. PCA, etc). For time-consuming computations, you can see the progress of the computations displayed as colored squares in a horizontal bar at the bottom of the dialog.

Dialog: Progress (here in the case of PCA)



While the computations are going on, a Cancel button allows you to stop the computations.

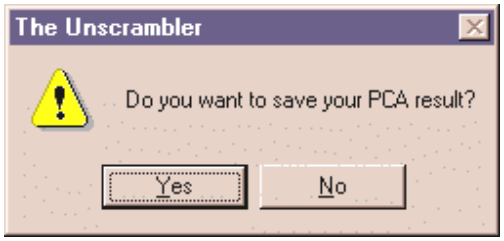
For projection methods (PCA, PCR, PLS) the **Progress** dialog also displays the relevant residual variance after each PC.

When the bar is full, the computations are finished and two new buttons appear at the bottom.

Select View to display the results in the Viewer.

Select Close if you do not want to view the results now. A warning dialog pops up, prompting you for saving the results file.

Dialog: "Do you want to save?" upon clicking Close in Progress dialog



Choosing Yes in this dialog has the same effect as selecting **File - Save As...** when the results file is opened in the Viewer.

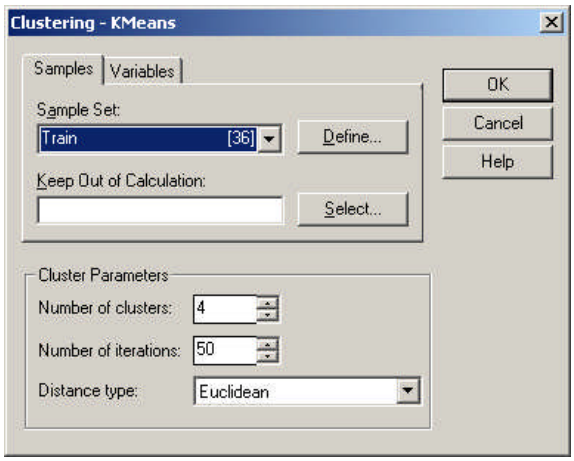
If you choose No, the results are lost and can only be re-created by running the same task once again.

Task - Clustering...

Launches an unsupervised classification of samples using the K-means clustering method. The samples will be grouped into K (user-determined number) clusters based on a specific distance measurement, so that the sum of distances between each sample and its cluster centroid is minimized.

In the **Clustering** dialog, you can specify the technical details of the computations.

Dialog: Clustering - KMeans



General Options

In the **Cluster Parameters** frame at the bottom of the dialog box, you specify the Number of clusters the samples should be divided into, and the Number of iterations to be performed before the results are displayed.

Select the Distance type to be used for the clustering procedure. The drop-down list allows you to choose from the following:

- Euclidean distance:
  This is the most usual, "natural" and intuitive way of computing a distance between two samples. It takes into account the difference between two samples directly, based on the magnitude of changes in the sample levels.
  This distance type is usually used for data sets that are suitably normalized or without any special distribution problem.
- Manhattan distance:
  Also known as city-block distance, this distance measurement is especially relevant for discrete data sets. While the Euclidean distance corresponds to the length of the shortest path between two samples (i.e. "as the crow flies"), the Manhattan distance refers to the sum of distances along each dimension (i.e. "walking round the block").
- Pearson Correlation distance:
  This distance is based on the Pearson correlation coefficient that is calculated from the sample values and their standard deviations. The correlation coefficient takes values from –1 (large, negative correlation) to +1 (large, positive correlation).
  Effectively, the Pearson distance lies between 0 (when correlation coefficient is +1, i.e. the two samples are most similar) and 2 (when correlation coefficient is -1).
  Note that the data are centered by subtracting the mean, and scaled by dividing by the standard deviation.
- Absolute Pearson Correlation distance:
  In this distance, the absolute value of the Pearson correlation coefficient is used; hence the corresponding distance lies between 0 and 1, just like the correlation coefficient.
  Taking the absolute value gives equal meaning to positive and negative correlations, due to which anti-correlated samples will get clustered together.
- Un-centered Correlation distance:
  This is the same as the Pearson correlation, except that the sample means are set to zero in the expression

for un-centered correlation. The un-centered correlation coefficient lies between –1 and +1; hence the distance lies between 0 and 2.

- Absolute, Un-centered Correlation distance:
  This is the same as the Absolute Pearson correlation, except that the sample means are set to zero in the expression for un-centered correlation. The un-centered correlation coefficient lies between 0 and +1; hence the distance lies between 0 and 1.
- Kendall's (tau) distance:
  This non-parametric distance measurement is more useful in identifying samples with a huge deviation in a given data set.

Note: If the data set contains any sample with a standard deviation of zero (i.e. no variation among its variables), the 4 correlation methods should be avoided.

Once you are satisfied with your choices, hit OK.

The clustering results are displayed in the data table as a Category variable called "<Distance type>_SOD <value of sum of distances>", containing the ID (1, 2, …, N) of the cluster each sample has been affected to.

For instance, if the clustering was performed using the Euclidean distance, and the best result (the one now displayed in the data table) after 50 iterations was a sum of distances of 80.7654, then the clustering variable is called "Euclidean_SOD 80.7654".

Clustering Dialog: Samples Sheet

Choose the Sample Set on which you want to base the calculations from the Sample Set drop-down list. The K-means clustering will be performed for the entire chosen sample set. If you want to define a new set, click Define to launch the **Set Editor** dialog.

If you want to exclude some of the samples from the analysis, type in their numbers in the field Keep Out of Calculation, or click Select to choose them directly from an Editor (the **Select Samples** dialog). Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27.

Clustering Dialog: Variables Sheet

On the Variables sheet you decide on which Variable Set to perform the calculations in the Variable Set field. Only continuous variables may be chosen. If there are any category variables in your selection, they will be automatically excluded from the analysis. To define new variable sets, click Define to go to the **Set Editor**.

If you want to exclude some of the variables from the analysis, type in their numbers in the field Keep Out of Calculation, or click Select to choose them directly from an Editor Editor (the **Select Variables** dialog). Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27.

Clustering Dialog: Sum Of Distances and Number of Iterations

The ***K-Means clustering algorithm*** consists of the following three steps:

1. The algorithm is initiated by creating 'k' different clusters. The sample set included in the analysis is first randomly distributed between these 'k' different clusters.
2. As a next step, the distance between each sample and its respective cluster centroid is calculated.
3. Samples are then moved to a cluster (k') that records the shortest distance from each sample to the cluster centroid.

The ***Number of Iterations*** is the number of times the K-Means algorithm is repeated to obtain an optimal clustering solution, every time starting with random initial clusters.

The ***Sum of Distances (SOD)*** is described as the sum of the distance values of each sample to their respective cluster centroid, summed up over all 'k' clusters. This parameter is uniquely calculated for each batch of cluster-IDs resulting from one single iteration of the algorithm. The results from all iterations are compared, and the solution with least SOD is retained.

Recommended Procedure for Clustering

Start the analysis with a small Number of Iterations, say for example 10 if the sample set contains 500 samples. After obtaining the first clustering results, keep the clustering variable in the data table and launch a new analysis with a larger Number of Iterations; this should normally result in a solution with a lower SOD (if not, try again a few times before giving up). Go on running new analyses with increasing Number of Iterations until you no get no more improvement on the resulting SOD. **Pick the clustering variable with the lowest SOD as your final result**.

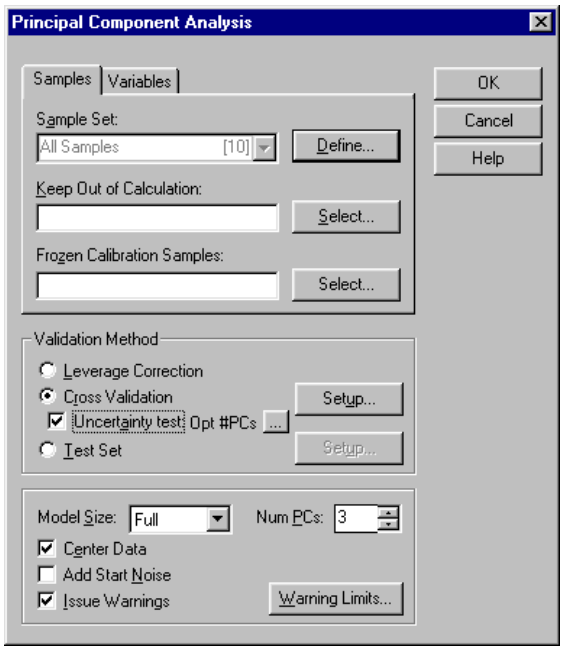
Note: Since the first step of the K-Means algorithm is based on the random distribution of the samples into 'k' different clusters there is a good possibility that the final clustering solution will not be exactly the same for every instance for a fairly large sample data set.

Task - PCA...

In the **Principal Component Analysis** dialog, you define the data on which the model will be based, the maximum complexity of the model, and how to validate the model.

The dialog contains two sheets: Samples and Variables, and two general groups of options: Validation Method and some miscellaneous options.

Dialog: Principal Component Analysis



PCA Dialog: Samples Sheet

Choose the Sample Set on which you want to base the calculations from the Sample Set drop-down list. The analysis is performed on the entire chosen sample set. If you want to define a new set, click Define to launch the **Set Editor** dialog.

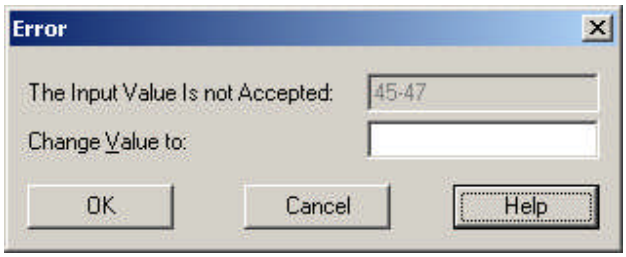
If you want to exclude some of the samples from the analysis, type in their numbers in the field Keep Out of Calculation, or click Select to choose them directly from an Editor (the **Select Samples** dialog). Ranges are indicated by hyphens and different ranges are separated by commas, for example: 1-5,7,10-13,27.

Note** - How to use **Sample Set** and **Keep Out:

- In Sample Set you select the general sample "population" the analysis applies to.
- In Keep Out… you remove one (or more) of these samples if it turns out that they disturb the results.

Note: Invalid sample range in the Keep Out field will result in an error message, as shown below:

Error message upon invalid sample range



In the field Frozen Calibration Samples you may type in the list of frozen samples directly, or press Select to enter an Editor where you can select the appropriate samples.

This field is only enabled if you have chosen the validation method Cross Validation. The frozen samples are always used in the calibration and are never included in any test sets. Thus, they can be regarded as especially important in the analysis.

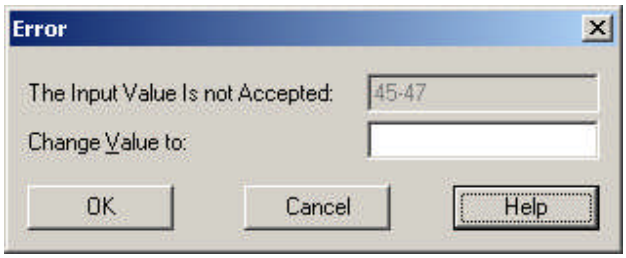
PCA Dialog: Variables Sheet

Choose which variables to use in your calculation in the Variable Set field. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you enter by clicking Define.

In the Keep Out of Calculation field you enter any variables which you do not want to include in the analyses, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27. This does not delete the variables from the set, it merely makes a model without them. Press Select to enter an Editor where you can select the variables to omit. Result matrices include entries for the omitted variables, but the value for these entries will be defined as "missing".

Note: Invalid variable range in the Keep Out field will result in an error message, as shown below:

Error message upon invalid variable range



You can also choose to include interaction and square effects in the calculation by pressing the button I&S, which launches the **Interaction and Square Effects Selection** dialog.

You also need to define the Weights for your variables in the **Set Weights** dialog. The weighting determines the role of each of the variables; you can change their influence on the model. Consider weighting = 1/SDev if you want all variables to have equal chances to influence the model.

PCA Dialog: Validation Methods

Validation is important to check whether your model will make a good fit on future data not used in the original computations. A good model should generally describe data similar to that available when building the model. Validation gives you an estimate of the error you can expect when fitting new, similar data to the model. It is also important when determining how many components are optimal for the data at hand.

In the Validation method field you choose between the 3 provided options as listed below.

Note: Be cautious when you have a designed data table. Do not use Cross Validation when there are few samples in the data table.

Validation methods

Validation method	Description
Leverage Correction	"Quick and dirty". Used for a rough, initial estimate. Do not use it for final validation as the leverage correction validation results are often too optimistic.
Cross Validation	Simulates test set validation. May be time consuming. Allows you to use Martens' Uncertainty test.
Test Set	Validates the model against separate samples.

If you choose the method Cross Validation the Setup button next to it will be enabled. Press it to enter the **Cross Validation Setup** dialog, where you can further define your cross validation settings.

Tick in the box for Uncertainty Test (only active if Cross Validation has been selected) if you wish to take advantage of cross validation segments for assessing the stability of your results (***Martens' Uncertainty Test***).

Tick the button ... to access the **Uncertainty Test** dialog, where you can set up the number of PCs to use in the Uncertainty Test (this is ***not*** the same as the number of PCs computed in your analysis).

If you choose the validation method Test Set, press Setup to enter the **Test Set Validation Setup** dialog, where you can further define your test set validation settings.

PCA Dialog: Miscellaneous Options

In the bottom of the dialog you can find general options for your analysis:

1. Model Size;
2. Number of PCs to be computed;
3. Center Data;
4. Add Start Noise;
5. Issue Warnings.

Number of PCs

In the Num PCs field, you define the maximum number of Principal Components to compute. Choosing many components will give you a model which explains more of the variations in the data, but which also takes more time to build.

For a first computation we recommend that you choose a rather large number of PCs (1/2 or 1/3 of the total number of X-variables for non-spectral data, around 10 for spectra) so as not to miss the optimum in the variance curve. Later on, you may re-calculate your model with fewer components (e.g. one more than the optimal number, so that the optimum still shows on the variance curve) to limit the size of the model.

Model Size

From the combo-box, choose between the three possible model sizes: Full, Compact and Minimum.

- The Full model (which is the default) contains all possible result matrices, and thus can be opened in a Viewer and used in Prediction and/or Classification (on-line or off-line).
- The Compact model excludes the following result matrices from the model: *Eix (X-residuals)*, *Fiy (Y-residuals)*, *xWeighted* and *yWeighted (weighted raw X and Y variables)*. The Compact models have the same applicability as the Full models.
- The Minimum model only contains the result matrices needed for the Prediction and Classification analyses to work. In addition, three very small matrices (they each only contain a vector of size A, the number of principal components) are included in order to maintain useful functionality in the file dialogs; the variance plot, the variance details dialog and the print details mechanism. Preserving this functionality helps assessing the model quality when opening models for Prediction or Classification via file dialogs.

Note: Restrictions on the Minimum Model

The Minimum model does not contain enough result matrices to be opened in a Viewer. When the calibration is finished the **View** button is hidden, making the **Close** button the only allowed action in the **Progress** dialog. When clicking this button, you are asked to save the model as usual. Later on, if you try to open the model from the **File-Open** or **Results** dialog, a message will pop up, informing you that the model cannot be viewed.

The limited number of result matrices in a Minimum model also has some effect on the **Export Model** functionality. For Minimum models this option is only available by selecting a model in the **Results** dialog and clicking the **Export** button. For a Minimum PCA model only the Tracker format is supported.

Center Data

Ticking the Center Data box makes a model where the data have been centered first, i.e. the average of each variable is subtracted from each of the data values in the variable.

Centering means that the results can be interpreted in terms of deviations from the average; this option is highly recommended. You should have a good reason for choosing not to center your data before an analysis.

Add Start Noise

You can select Add Start Noise if you want noise to be added to your data before the analysis is performed. This option should only be used in special situations where a special data distribution makes it difficult for the algorithms to find a start direction.

Issue Warnings

Finally, The Unscrambler can give you warnings for several situations which may indicate poor validity of the results, if you tick the Issue Warnings box. For example, the program can detect high leverages, outliers in sample and variable space, unusually low total explained variance, etc.

The warnings are issued in accordance to the specifications in the **Warning Limits** dialog, which you enter by clicking the Warning Limits button.

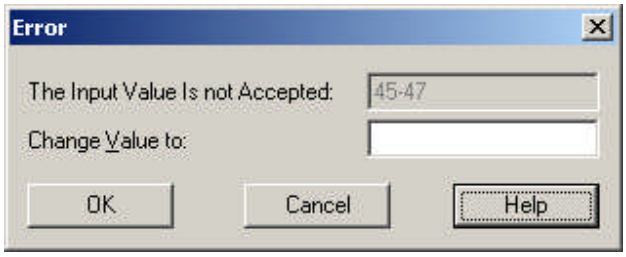
Note: Remember that warnings are time and memory consuming. Turn them off if you do not intend to use them.

Invalid Sample or Variable Range

In all analysis dialogs (Statistics, PCA, Regression, etc.) you have the possibility to specify samples or variables to be kept out of the calculations. The range for those samples or variables may be entered either using an Editor through the Select button, or directly.

Upon direct entry, you may get an error message if the range you specified is invalid with respect to the samples (or variables) present in the Sample set (or Variable set) to be analyzed.

Error message upon invalid sample or variable range



Should this dialog show up, type in a new range, within the range of samples (or variables) present in the current Sample set (or Variable set).

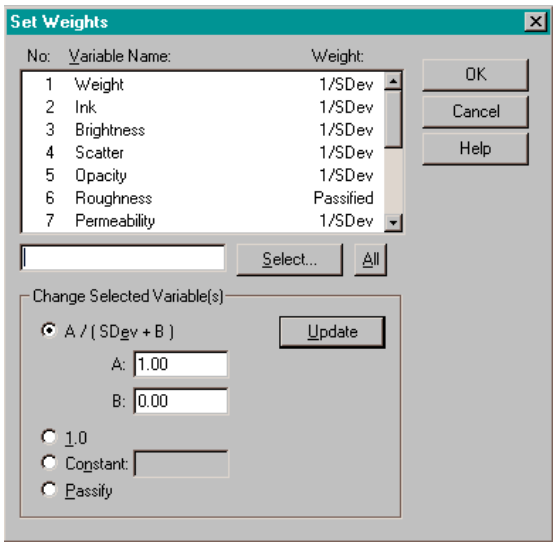
If you do not remember the correct range, click Cancel to return to the analysis dialog, and use the Select button to select a valid range.

Set Weights Dialog

PCA, PLS and PCR analyses depend on the relative standard deviation of the variables. For PLS2, both X- and Y-variables can be weighted so that only the relative differences among the variance of the X-variables and the relative differences among the Y-variables influence the model.

When you press the Weights button in a dialog, you launch the **Set Weights** dialog.

Dialog: Set Weights



How To Use the Set Weights Dialog

1. First, select the variables for which you want to set the weights in the top field. You can either enter the number(s) of the variable(s) for which you want to change the weight(s) in the box below the list, press Select to enter an Editor where you can find the variables you are looking for, or press All to select all variables.
2. Then you choose the appropriate weighting for the selected variables in the Change Selected Variable(s) field ***and press*** Update ***to update the selected weights in the list***.

The following weighting options can be chosen from the Change Selected Variable(s) field at the bottom of the dialog:

- A(Sdev + B)
- 1.0
- Constant
- Passify

A/(Sdev + B)

The weighting A/(SDev + B) with ***A = 1.0 and B = 0.0*** (i.e. ***1/Sdev***) is called ***standardization*** and is used to give all the variables the same variance (= 1). If this is used, all the variables are given the same chance to influence the estimation of the components. This is often used if the variables

1. are measured with different units;
2. have different ranges;
3. are of different types.

Sensory data are sometimes standardized if the scales of the different attributes vary greatly. Spectra are usually not standardized.

Note: If noisy variables with small standard deviation are standardized their influence is exaggerated, which can sometimes make the model less reliable.

Using constants other than A = 1.0 and B = 0.0 gives you the possibility to weight the variables with a combination of 1/SDev and a constant. This can be a useful compromise in cases where full standardization might be dangerous.

1.0

1.0 represents no weighting at all, i.e. all variables are used as they are.

Constant

Constant sets the weight to a constant number independently of the standard deviation.

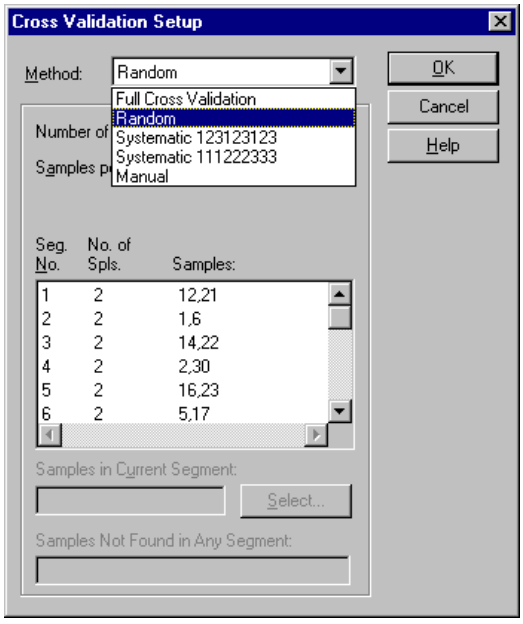
Passify

Passify sets the weight to a very small constant number, so that the variable loses all influence on the model but still appears in projection plots. Once you click Update, the variable appears as *Passified* in the list.

Cross Validation Setup Dialog

If you choose the method Cross Validation in a dialog the Setup button next to it will be enabled. Press this, and you enter the **Cross Validation Setup** dialog, where you can choose which cross validation method you want to use and the properties of that method.

Dialog: Cross Validation Setup



The drop-down Method menu gives you five different cross validation options to choose from. These are listed below.

Cross Validation methods

Method	Description
Full Cross Validation	There are as many segments as there are samples (one sample per segment). “Leave-one-out”.
Random	You select the number of segments or the number of samples per segment. The Unscrambler picks the samples at random.
Systematic 123123	You select the number of segments or the number of samples per segment. The first sample belongs to the first segment, the second sample to the second segment, etc.
Systematic 112233	You select the number of segments or the number of samples per segment. First N samples belong to the first segment, next N samples to the second segment, etc.
Manual	You select the number of segments or the number of samples per segment. The Unscrambler gives a suggestion for which samples belong to which segments. You can override this by changing the sample numbers. Every change you want to make has to be done manually through the box below the segment list. Any samples that have not been assigned to a segment are listed in the field “Samples not found in any segment”.

Select the Number of Segments you want in the cross validation, or how many samples there should be in each segment, in the appropriate fields. These two options are inter-dependent; any change you make in one is automatically reflected in the other.

The Samples in Current Segment box shows the sample numbers of the selected segment in the segment list. The box is opened for changes only when manual cross validation is selected.

Test Set Validation Setup Dialog

The Setup button in the Validation field in a dialog will also be enabled if you choose the validation method Test Set. Press Setup, and you enter the **Test Set Validation Setup** dialog. You can select the test set samples manually or by group, or let The Unscrambler pick them at random by choosing the appropriate radio button.

If you choose Manual Selection, enter the test set samples in the appropriate box or press Select to enter the **Set Editor** where you can easily choose the samples you want.

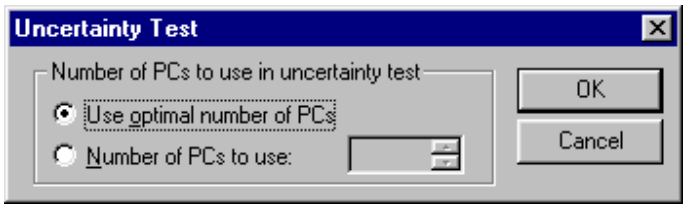
If the data table contains category variables, or if it is a designed data table, you may use Group Selection, i.e. a level as a test set. Select which variable you want to group by, and whether the test set should be equal to or differ from the level in the box to the right.

If you select Random selection, you only need to specify how many samples you want in the test set. The Unscrambler picks these at random from the set you are working with. A new random selection of test samples is made each time a new analysis is run.

Uncertainty Test Dialog

You can either decide how many Principal Components should be taken in consideration during the rotation or let The Unscrambler use the optimal number. This selection is done by clicking on the button shown hereafter:

Dialog: Uncertainty Test



How To Select Number of PCs to Use

We suggest that you make a first model, then remove obvious outliers, and interpret results from the new model to find the optimal number of components to be used in the Uncertainty Test.

Make sure to look at individual Y-variances in PLS2 situations. The optimum number of PCs (PLS components) may be varying for the different Y-Variables. Individual PLS1 models often have better prediction ability than a global PLS2 model, unless the Y-variables are collinear.

Warning Limits Dialog

During analysis, a number of tests are applied to the results. If the values calculated during these tests fall outside certain limits, a warning is issued. These limits are user-definable, i.e. you can change them by selecting Warning Limits in the appropriate **Task** dialog, thus entering the **Warning Limits** dialog. The default limits are, to a certain extent, heuristic and derived from past experience.

There is no such thing as “correct” limits; limits are only filters used to highlight the “most extreme” results of each test.

The actual value of a useful limit may vary from one application to another. If you get too many warnings, raise the limit. On the other hand, if you get few warnings even though you know there are outliers, decrease the limit. Limits of 4-5 are usual for spectroscopy data.

Note: All limits do not apply to every analysis. Only those that apply to the analysis you are about to perform are shown in this dialog.

The options in the **Warning Limits** dialog are listed and described below.

Warning limits

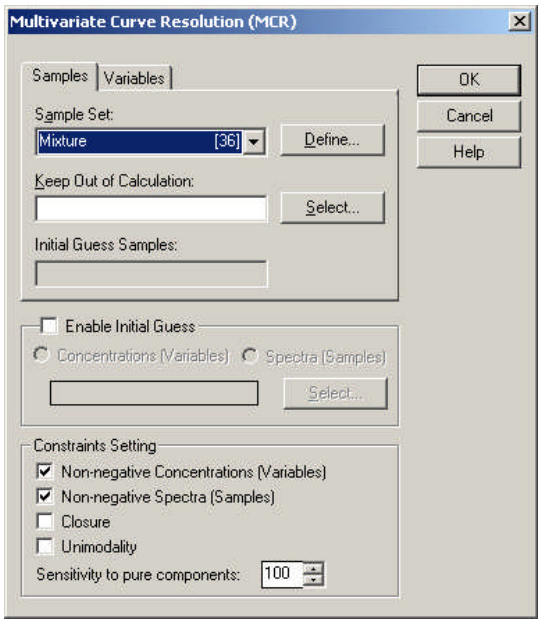
Limit	Description
Leverage Limit	Objects with high leverage have a large influence on the model and may be dangerous if erroneous.
Ratio of Calibrated to Validated Explained Variance	Calibration set may lack representativity.
Ratio of Validated to Calibrated Explained Variance	Indicates an unstable structure in the model or that outliers may be present.
Ratio of Calibrated to Validated Multiple Correlation	Calibration set may lack representativity.
Ratio of Validated to Calibrated Multiple Correlation	Validation set may lack representativity.
Sample Outlier Limit, Calibration	Some samples are badly fitted.
Sample Outlier Limit, Validation	Some samples are badly fitted.
Statistical Condition Number	The X-matrix is ill-conditioned, and it may be difficult to estimate the model parameters.
Total Explained Variance (%)	The model does not describe the data well.
Variable Outlier Limit, Calibration	Some variables are badly fitted.
Variable Outlier Limit, Validation	Some variables are badly fitted.

Task - MCR...

In the **Multivariate Curve Resolution (MCR)** dialog, you define the data on which the model will be based and specify the technical features of the computations.

The dialog contains two sheets: Samples and Variables, and two general groups of options: Enable Initial Guess and Constraints Setting.

Dialog: Multivariate Curve Resolution (MCR)



MCR Dialog: Samples Sheet

In the Sample Set field, select the sample set on which to perform the calculations. Use Keep Out of Calculation if you wish to leave out some of the samples. If you have enabled an initial guess based on some known spectra, the corresponding sample numbers are displayed in the Initial Guess Samples field.

For more details on how to use the Define and Select buttons, you may lookup the description of a similar sheet in PCA Dialog: Samples Sheet p.259.

MCR Dialog: Variables Sheet

In the Variable Set field, select the variable set on which to perform the calculations. Use Keep Out of Calculation if you wish to leave out some of the variables. If you have enabled an initial guess based on some known concentrations, the corresponding variable numbers are displayed in the Initial Guess Variables field.

For more details on how to use the Define and Select buttons, you may lookup the description of a similar sheet in PCA Dialog: Samples Sheet p.259.

MCR Dialog: Enable Initial Guess

This field allows you to take into account any prior information you may have on the mixture constituents.

Initial Guess for Concentrations

Use this option if some of the variables in the data table contain known concentrations of the mixture constituents – or an approximation of those concentrations.

Type in the variable range directly or click Select to select relevant columns from an Editor window. The corresponding variable numbers will be updated in the Initial Guess Variables field of the Variables sheet.

Initial Guess for Spectra

Use this option if some of the samples in the data table are known to be pure constituent spectra, or assumed to be an approximation of those.

Type in the sample range directly or click Select to select relevant rows from an Editor window. The corresponding sample numbers will be updated in the Initial Guess Samples field of the Samples sheet.

Note: Variables (resp. samples) defined as "Initial Guess" cannot be part of the model data. In case of overlap, an error message appears when you launch the computations, as shown hereafter:

To fix the problem, remove the offending variables / samples from the model data by typing in their range in the Keep Out of Calculation field.

MCR Dialog: Constraints Setting

This group of options specifies the constraints to be taken into account in the model. The following choices are available:

- Non-negative Concentrations (Variables) is selected by default. This is the most common case.
- Non-negative Spectra (Samples) is selected by default. In many applications the instrumental measurements, e.g. UV absorbance or fluorescence intensity, can be assumed to be non-negative.
- Closure is not selected by default. Choose this option if you have reason to assume that the sum of the concentrations is constant over all samples.
- Unimodality is not selected by default. Choose this option if you want to allow for only one maximum per profile. This is the case for instance for chromatograms.
- Sensitivity to pure components has a default value of 100. You may tune this value up or down between 10 and 190 by increments of 10.
  This parameter has an effect on the convergence properties of the algorithm. When later viewing your MCR results, you will have the possibility to display an MCR Message List recommending changes in Sensitivity whenever necessary to improve the results.

  Note that this option is disabled if you have enabled Initial Guess.

Task - Regression...

Launches a dialog that allows you to set up the details of your regression model.

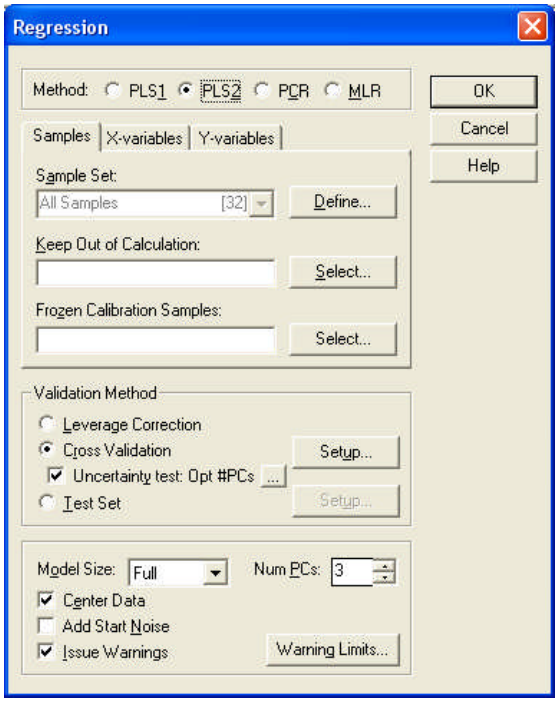
Depending on the nature of the data table displayed in the Editor upon choosing **Task - Regression**, the following dialog is accessed:

- For a regular (2-D) data table, the **Regression** dialog shown hereafter allows you to specify a regression model of type PLS1, PLS2, PCR or MLR;
- For a 3-D data table, the **Regression (Three-Way PLS)** dialog allows you to specify a tri-PLS (nPLS) regression model. This dialog is described in section Regression (Three-Way PLS) Dialog.

Note: What follows applies to 2-D data only.

In the **Regression** dialog you can set up which data the model will be based on, the maximum complexity of the model, and how to validate the model.

Dialog: Regression



First, select the appropriate regression method for your problem and type of data in the Method field. The available methods are described below.

Regression methods

Regression Method	Description
PLS1 (**P**artial **L**east **S**quares Regression)	This method is valid in all situations, especially if there is some correlation among your X-variables. It builds a model with only 1 Y-variable.
PLS2 (**P**artial **L**east **S**quares Regression)	This method is valid in all situations, especially if there is some correlation among your X-variables. It models several Y-variables together, which is useful if there is some correlation among your Y-variables.
PCR (**P**rincipal **C**omponent **R**egression)	This method is an alternative to PLS1. It runs an MLR on the principal components of X. Several Y-variables can be modeled individually (you get results for all Y-variables in one run, but the results are based on separate models).

MLR: (**M**ultiple **L**inear **R**egression)	This method should only be used when the X-variables are not correlated or have only a small correlation. One model is made per Y-variable.

Next, you must specify which Sample and Variable Sets to use on the Samples, X- and Y-Variables sheets respectively. The Samples sheet is identical for all the methods, while the X- and Y-Variables sheets and the common options at the bottom of the dialog differ slightly for PLS or PCR on one side and MLR on the other side.

Regression Dialog: Samples Sheet

In the Sample Set field, select the sample set on which to perform the calculations. Use Keep Out of Calculation if you wish to leave out some of the samples. Finally, define the Frozen Calibration Samples in the corresponding field.

For more details, you may lookup the description of a similar sheet in PCA Dialog: Samples Sheet p.259.

Regression Dialog: X-Variables Sheet and Y-Variables Sheet (PLS and PCR)

On both sheets, choose which variables to use in your calculation in the Variable Set field. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you enter by pressing Define.

In the Keep Out of Calculation field you enter any variables which you do not want to include in the analysis, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27.

On the X-variables sheet you can also choose to include interaction and square effects in the calculation by pressing the button I&S, which launches the **Interaction and Square Effects Selection** dialog.

On both sheets, you also need to define the Weights for your variables in the **Set Weights** dialog. The weighting determines the role of each of the variables; you can change their influence on the model. Consider weighting = 1/SDev if you want all variables to have equal chances to influence the model.

Note: You cannot have the same variable in both the X-variable and the Y-variable set.

Regression Dialog: X-Variables Sheet and Y-Variables Sheet (MLR)

These sheets are essentially identical to the sheets for PLS1, PLS2 and PCR, but for MLR, the weights are set to All 1.0 by default. This means that the Weights button is disabled.

Note: You cannot have the same variable in both the X-variable and the Y-variable set.

Regression Dialog: Validation Methods (PLS and PCR)

Validation is important to check whether your model will make a good fit on future data not used in the original computations. A good model should generally describe data similar to that available when building the model. Validation gives you an estimate of the error you can expect when fitting new, similar data to the model. It is also important when determining how many components are optimal for the data at hand.

In the Validation method field you choose between the 3 provided options as listed below.

Note: Be cautious when you have a designed data table. Do not use Cross Validation when there are few samples in the data table.

Validation methods

Validation method	Description
Leverage Correction	"Quick and dirty". Used for a rough, initial estimate. Do not use it for final validation as the leverage correction validation results are often too optimistic.
Cross Validation	Simulates test set validation. May be time consuming. Allows you to use Martens' Uncertainty test.
Test Set	Validates the model against separate samples.

If you choose the method Cross Validation the Setup button next to it will be enabled. Press it to enter the **Cross Validation Setup** dialog, where you can further define your cross validation settings.

Tick in the box for Uncertainty Test (only active if Cross Validation has been selected) if you wish to take advantage of cross validation segments for assessing the stability of your results (***Martens' Uncertainty Test***).

Tick the button to access the **Uncertainty Test** dialog, where you can set up the number of PCs to use in the Uncertainty Test (this is ***not*** the same as the number of PCs computed in your analysis).

If you choose the validation method Test Set, press Setup to enter the **Test Set Validation Setup** dialog, where you can further define your test set validation settings.

Regression Dialog: Miscellaneous Options (PLS and PCR)

In the bottom of the dialog you can find general options for your analysis:

1. Model Size;
2. Number of PCs to be computed;
3. Center Data;
4. Add Start Noise;
5. Issue Warnings.

Number of PCs

In the Num PCs field, you define the maximum number of Principal Components to compute. Choosing many components will give you a model which explains more of the variations in the data, but which also takes more time to build.

For a first computation we recommend that you choose a rather large number of PCs (1/2 or 1/3 of the total number of X-variables for non-spectral data, around 10 for spectra) so as not to miss the optimum in the variance curve. Later on, you may re-calculate your model with fewer components (e.g. one more than the optimal number, so that the optimum still shows on the variance curve) to limit the size of the model.

Model Size

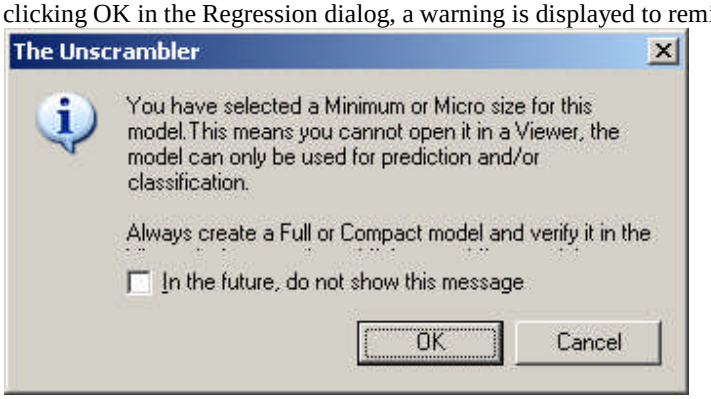
From the combo-box, choose between the three possible model sizes: Full, Compact and Minimum.

- The Full model (which is the default) contains all possible result matrices, and thus can be opened in a Viewer and used in Prediction and/or Classification (on-line or off-line).
- The Compact model excludes the following result matrices from the model: *Eix (X-residuals)*, *Fiy (Y-residuals)*, *xWeighted* and *yWeighted (weighted raw X and Y variables)*. The Compact models have the same applicability as the Full models.

- The Minimum model only contains the result matrices needed for the Prediction and Classification analyses to work. In addition, three very small matrices (they each only contain a vector of size A, the number of principal components) are included in order to maintain useful functionality in the file dialogs; the variance plot, the variance details dialog and the print details mechanism. Preserving this functionality helps assessing the model quality when opening models for Prediction or Classification via file dialogs.
- The Micro model is the smallest possible; it can only be used for Prediction. To limit model size even more than with the Minimum model, the results matrices are saved for the maximum number of PCs only (i.e. PCmax). This means that at the Prediction stage, the number of PCs to use will be frozen to PCmax.

Note: Restrictions on the Minimum and Micro Models

The Minimum and Micro models do not contain enough result matrices to be opened in a Viewer. Upon clicking OK in the Regression dialog, a warning is displayed to remind you of the restrictions, as shown below:


The Unscrambler
You have selected a Minimum or Micro size for this model.This means you cannot open it in a Viewer, the model can only be used for prediction and/or classification.
Always create a Full or Compact model and verify it in the
In the future, do not show this message
OK
Cancel

When the calibration is finished the **View** button is hidden, making the **Close** button the only allowed action in the **Progress** dialog. When clicking this button, you are asked to save the model as usual. Later on, if you try to open the model from the **File - Open** or **Results** dialog, a message will pop up, informing you that the model cannot be viewed.

The limited number of result matrices in models of reduced size also has some effect on the **Export Model** functionality. For Minimum and Micro models this option is only available by selecting a model in the **Results** dialog and clicking the **Export** button. For a Minimum PCA model, only the Tracker format is supported. For a Minimum regression model, ASCII-MOD and Tracker are supported. For a Micro regression model, only ASCII-MOD is supported.

Minimum and Micro models support ***automatic pre-treatment*** at the Prediction (or Classification, Minimum only) stage. Use the **Results** dialog and click the **Properties** button to register the transformations for automatic pre-treatment.

Warning:

You should select model size "Micro" only after having computed and validated a similar model with size "Full" or "Compact". Use the optimal number of PCs determined from that previous model as Num PCs (total number of PCs to be computed) for the Micro model. This way, you will ensure use of the correct number of PCs at the Prediction stage.

Center Data

Ticking the Center Data box makes a model where the data have been centered first, i.e. the average of each variable is subtracted from each of the data values in the variable.

Centering means that the results can be interpreted in terms of deviations from the average; this option is highly recommended. You should have a good reason for choosing not to center your data before an analysis.

Add Start Noise

You can select Add Start Noise if you want noise to be added to your data before the analysis is performed. This option should only be used in special situations where a special data distribution makes it difficult for the algorithms to find a start direction.

Issue Warnings

Finally, The Unscrambler can give you warnings for several situations which may indicate poor validity of the results, if you tick the Issue Warnings box. For example, the program can detect high leverages, outliers in sample and variable space, unusually low total explained variance, etc.

The warnings are issued in accordance to the specifications in the **Warning Limits** dialog, which you enter by clicking the Warning Limits button.

Note: Remember that warnings are time and memory consuming. Turn them off if you do not intend to use them.

Regression Dialog: Miscellaneous Options (MLR)

In the field Validation Method, you can choose between the following validation methods:

1. Leverage Correction;
2. Full Cross Validation;
3. Test Set Validation.

Exercise caution when you have a designed data table. Do not use Full Cross Validation if your model is based on very few samples. Since the only cross validation method available for MLR is Full Cross Validation, the Setup button is disabled for this option.

Note: It is dangerous to use leverage correction in connection with MLR if the rank of any submatrix is different from the rank of the whole matrix, as the results cannot be trusted. Run MLR with cross validation first and see whether you get a warning that this is the case. If not, you may use leverage correction on later models with the same data selection to save time.

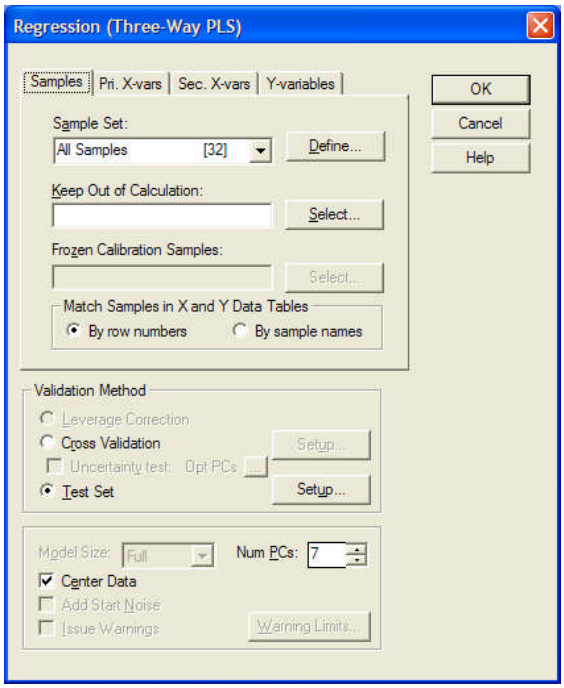
If you choose the validation method Test Set, press Setup to enter the **Test Set Validation Setup** dialog, where you can further define your test set validation settings.

In the bottom field of the dialog you define whether warnings should be issued by ticking or unticking the Issue Warnings box. Ticking it will enable the Warning Limits button, which launches the **Warning Limits** dialog.

Regression (Three-Way PLS) Dialog

The **Regression (Three-Way PLS)** dialog allows you to set up the details of your tri-PLS (nPLS) regression model.

Dialog: Regression (Three-Way PLS)



The top of the dialog lets you specify which Sample and Variable Sets to use on the Samples, Pri. X-vars, Sec. X-vars and Y-Variables sheets respectively.

The bottom of the dialog contains general options concerning the analysis: validation method, number of PCs, model centering.

Regression (Three-Way PLS) Dialog: Samples Sheet

Choose which samples to use in your calculation in the Sample Set field. You can either choose an existing Sample Set from the drop-down list or define a new in the **Set Editor**, which you access by pressing Define.

Then, specify any samples which you do not want to include in the analyses in the Keep Out of Calculation field, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27. You may also select samples to be kept out by clicking Select.

The next field allows you to specify how to Match Samples in X and Y Data Tables:

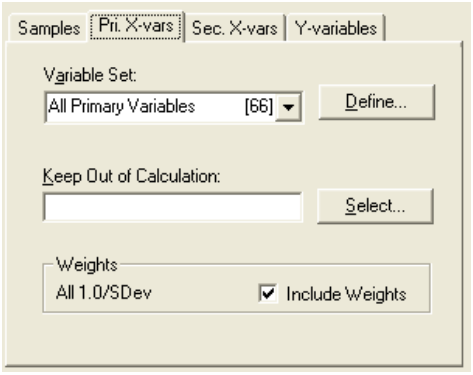
- By row numbers: the nth row of the 3D X-data table and the nth row of the 2D Y-data table are matched as one sample. This option requires that samples should be presented in the ***same order in both tables***.
- By sample names: The software matches the nth row of the 3D X-data table with whichever row of the Y-data table sharing the same sample name. This option allows for different sample randomisations in the two tables, but requires that each sample has ***a unique name***.

Note: the Frozen Calibration Samples option is disabled for tri-PLS.

Regression (Three-Way PLS) Dialog: Pri. X-vars Sheet and Sec. X-vars Sheet

These two sheets let you specify the Predictor variables in your tri-PLS model. Since they are stored in a 3-D array, Primary and Secondary X-variables are defined separately. As an example, the Pri. X-vars sheet is shown below.

Dialog: Regression (Three-Way PLS) - Pri. X-vars sheet



In the Variable Set field, choose which variables to use as Primary (resp. Secondary) X-variables. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you access by pressing Define.

In the Keep Out of Calculation field you enter any variables which you do not want to include in the analysis, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27. You may also select variables to be kept out by clicking Select.

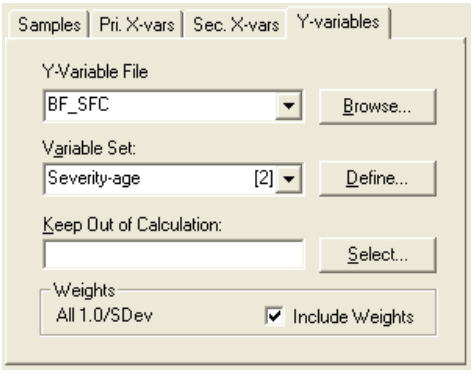
Weighting is done in the Weights field. Only 1/SDev is available as weighting option; you select it (for all X-variables) by ticking Include Weights.

Read more about weighting of 3-D arrays in Chapter "Centering and Weighting for Three-way Data".

Regression (Three-Way PLS) Dialog: Y-variables Sheet

This sheet lets you specify the Response variables in your tri-PLS model.

Dialog: Regression (Three-Way PLS) – Y-variables sheet



Since the 3-D data table displayed in the Editor upon launching **Task - Regression** only contains the X-variables, you have to get the Y-variables from another file (containing 2-D data). Use the Browse button to find the adequate Y-variable file.

In the Variable Set field, choose which variables to use as Y-variables. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you access by pressing Define.

In the Keep Out of Calculation field you enter any variables which you do not want to include in the analysis, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27. You may also select variables to be kept out by clicking Select.

Weighting is done in the Weights field. Only 1/SDev is available as weighting option; you select it (for all Y-variables) by ticking Include Weights.

Regression (Three-Way PLS) Dialog: General Options

In the bottom of the dialog you can find general options for your analysis:

1. Model Size;
2. Number of PCs to be computed;
3. Center Data;
4. Add Start Noise;
5. Issue Warnings.

Number of PCs

In the Num PCs field, you define the maximum number of Principal Components to compute. Choosing many components will give you a model which explains more of the variations in the data, but which also takes more time to build.

For a first computation we recommend that you choose a rather large number of PCs (1/2 or 1/3 of the total number of X-variables for non-spectral data, around 10 for spectra) so as not to miss the optimum in the variance curve. Later on, you may re-calculate your model with fewer components (e.g. one more than the optimal number, so that the optimum still shows on the variance curve) to limit the size of the model.

Read more about choosing the number of PCs for tri-PLS in Section “Maximum number of components” from Chapter Three-Way Data Analysis.

Model Size

This option is disabled; Three-way PLS models can only be saved with ***full size***.

Center Data

Ticking the Center Data box makes a model where the data have been centered first, i.e. the average of each variable is subtracted from each of the data values in the variable.

Centering means that the results can be interpreted in terms of deviations from the average; this option is highly recommended. You should have a good reason for choosing not to center your data before an analysis.

Read more about centering of 3-D arrays in Chapter “Centering and Weighting for Three-way Data”.

Add Start Noise

This option is disabled for Three-way PLS models.

Issue Warnings

Finally, The Unscrambler can give you warnings for several situations which may indicate poor validity of the results. For example, the program can detect high leverages, outliers in sample and variable space, unusually low total explained variance, etc.

For Three-way PLS models, the Issue Warnings box is ticked by default and this option cannot be changed.

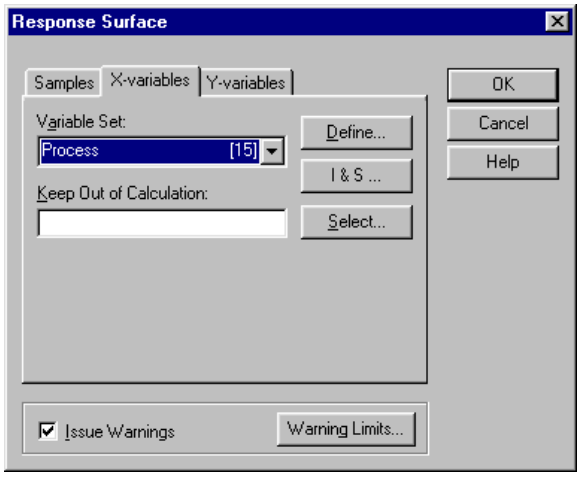
Task - Response Surface…

The **Response Surface** dialog is a dialog for polynomial regression analysis. On the three sheets in this dialog you set up which data the model will be based on, and how complex it will be.

The response surface gives a graphical picture of how the response (Y) depends on the predictor variables (X), their interactions and squares. It can be used for optimization, e.g. to find the settings of the predictor variables that give the optimal response. For non-designed data you can select subsets of samples to omit and decide which X-variables and Y-variables to use. For designed data, you can only choose which Y-variables to incorporate. The model can have any degree of complexity, from purely linear in the X-variables, to full quadratic (includes all interaction and square effects).

The dialog contains three sheets: ***Samples***, ***X-variables***, ***Y-variables***, as well as a ***Warnings*** field at the bottom.

Dialog: Response Surface



Warnings

In the bottom field of the dialog you define whether warnings should be issued by ticking or un-ticking the Issue Warnings box. Ticking it will enable the Warning Limits button, which launches the **Warning Limits** dialog.

Response Surface Dialog: Samples Sheet

Choose which samples to use in your calculation in the Sample Set field and enter any samples which you do not want to include in the analyses in the Keep Out of Calculation field.

For more details, you may lookup the description of a similar dialog in Statistics Dialog: Samples Sheet.

Response Surface Dialog: X-variables Sheet and Y-variables Sheet

In the Variable Set field you choose which Variable Set to use as X and Y respectively in the calculations. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you enter by clicking Define.

The computations can only be done for ***continuous*** variables. If there are category variables in the data selection, you must choose their level before computation starts. The category variable list box lists all the category variables. You will have to select one level for each variable by highlighting it in the list and then selecting one of its levels.

In the Keep Out of Calculation field you enter any variables which you do not want to include in the analyses, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27.

You can also choose to include interaction and square effects in the calculation by pressing the button I&S, which launches the **Interaction and Square Effects Selection** dialog.

At the bottom of the sheet, a list displays all Estimated Effects.

Note: You cannot have the same variable in both the X- and Y-variable set.

Task - Analysis of Effects...

The **Analysis of Effects** dialog is used to compute effects and test their significance (Analysis of Variance).

Analysis of Effects is only available for designed data tables.

The dialog contains three sheets: ***Samples***, ***X-variables***, ***Y-variables***, as well as a ***Warnings*** field at the bottom.

Warnings

In the bottom field of the dialog you define whether warnings should be issued by ticking or un-ticking the Issue Warnings box. Ticking it will enable the Warning Limits button, which launches the **Warning Limits** dialog.

Analysis of Effects Dialog: Samples Sheet

All design and reference samples are used for Analysis of Effect, hence the Sample Set field is frozen.

In the Keep Out of Calculation field you enter any samples which you do not want to include in the analyses, indicating ranges by hyphens and separating different ranges by commas, for example: 1-5,7,10-13,27.

For more details, you may lookup the description of a similar dialog in Statistics Dialog: Samples Sheet.

Analysis of Effects Dialog: X-variables Sheet and Y-variables Sheet

In the Variable Set field you choose which Variable Set to use as X and Y respectively in the calculations.

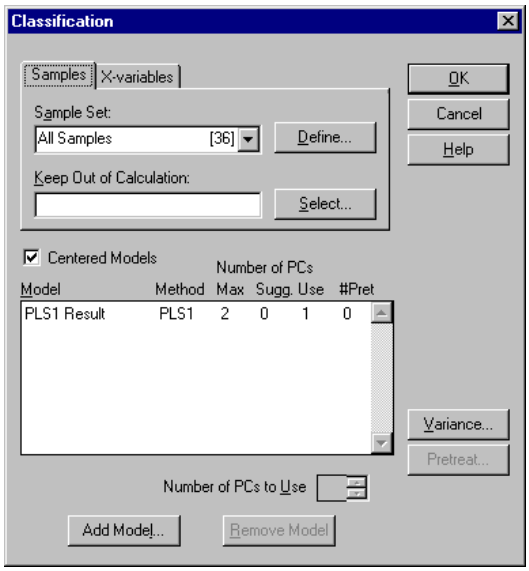
For more details, you may lookup the description of a similar dialog in Response Surface Dialog: X-variables Sheet and Y-variables Sheet.

Task - Classify...

The **Classification** dialog is used in the classification of new samples in comparison to existing, known models.

The dialog contains two sheets: ***Samples*** and ***X-variables***, as well as some ***general options*** at the bottom.

Dialog: Classification



Classification Dialog: Samples Sheet

Choose which samples to use in your calculation in the Sample Set field and enter any samples which you do not want to include in the analyses in the Keep Out of Calculation field.

For more details, you may lookup the description of a similar dialog in Statistics Dialog: Samples Sheet p.253.

Classification Dialog: X-variables Sheet

Here you choose which Variable Set to use as X in your calculation in the Variable Set field. You can either choose an existing Variable Set from the drop-down list or define a new in the **Set Editor**, which you enter by clicking Define.

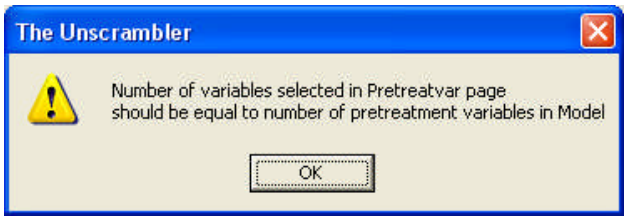
Classification Dialog: Pretreat Vars Sheet

This sheet is useful if you want to perform automatic pretreatments at the classification stage. Note that this option is only available if your class models have been calibrated on data pretreated in the Unscrambler.

Once you have selected relevant automatic pretreatments using the Pretreat button (see Classification Dialog: General Options), specify which Variable Set to pretreat, either by choosing an existing Variable Set from the drop-down list or by defining a new in the **Set Editor**, which you enter by clicking Define.

Note: You are free to select a Variable Set to pretreat which differs from the X-Variables set. But make sure that it contains the same number of variables as the original set of variables pretreated prior to building the class models. If not, you will get an error message as shown below.

Dialog: Invalid number of Pretreatment Variables


The Unscrambler
Number of variables selected in Pretreatvar page
should be equal to number of pretreatment variables in Model
OK

Classification Dialog: General Options

Tick the Centered Models box to make sure that only centered models are available for selection.

You select which models to use in the classification by pressing Add Model. This takes you to the **Get Model** dialog, where you can select the appropriate model. The number of X-variables must be the same in your new data and all models you use to classify it. SIMCA classification is only possible based on PCA, PCR, and PLS models. In the case of PCR and PLS models, only the X-part of the model will be taken into account.

Select each model in turn and specify how many PCs to use with the spin button. The Number of PCs to Use should be decided individually for each model you use in the classification. Your choice updates the number of PCs for this model in the classification dialog. A warning message is issued if you try to use more PCs than the optimal number suggested by The Unscrambler.

Press Variance to inspect the calibration and validation variances of the selected model. This takes you to the **Variance** Dialog, where the variances are shown for each PC in the selected model. Toggle between residual and explained variance by pressing the % button.

Use the Pretreat button to pretreat the model; this takes you to the **Select transformations** Dialog, where you may choose one or several of the pretreatments that were applied to the calibration data prior to building the class models. For an explanation of the abbreviations referring to various transformations, see the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

The Unscrambler suggests the optimal Number of PCs based on the residual variance curve. It chooses the first local minimum unless later PCs give significantly lower residual variance.

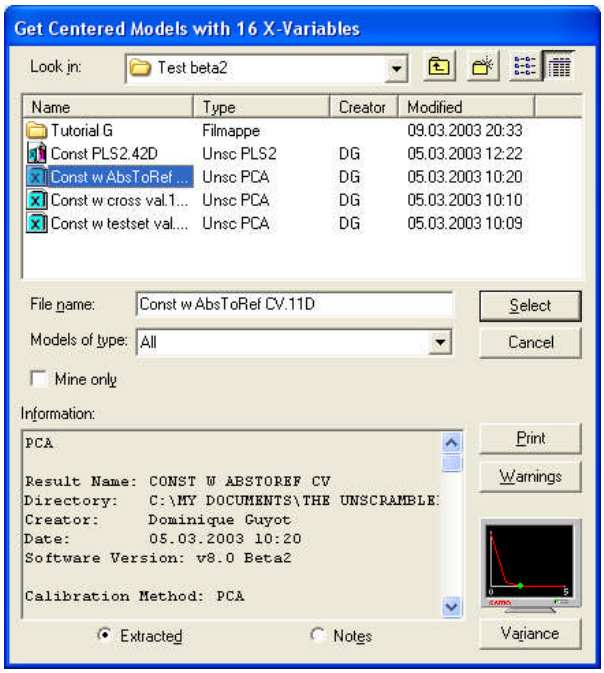
Note: Only models with exactly the same number of variables as in your new data selection will be shown in the Model window.

Get Model Dialog

This dialog is accessed either by clicking Add Model from the **Classification** dialog or Find from the **Prediction** dialog.

It allows you to locate a model with the relevant specifications (centered / uncentered, correct number of X-variables).

Dialog: Get Model (here in the case of Classification)



The relevant models stored in the current directory are displayed as a list. You may click your way to another directory if necessary.

If you wish to look for models of a specific type (e.g. PCA or PLS1), make your choice in the drop-down list of the field Models of Type.

If you wish to display only models that were created by yourself, tick the Mine only box.

Once a model has been selected in the list, more information and new buttons appear in the dialog to help you make your choice.

The Information field displays details about the contents of the selected model. It may be printed out with the Print button.

The Warnings button leads you to the **Text Warning List** dialog where you may lookup the wamings generated upon building the selected model.

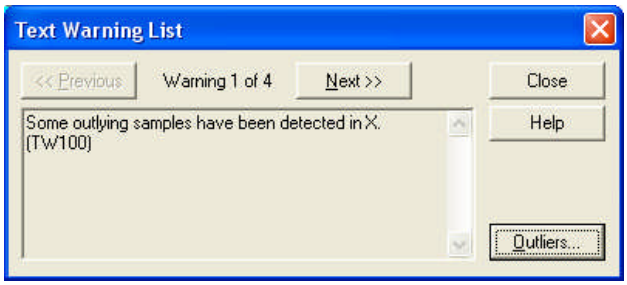
The Variance button leads you to the **Variance** dialog where you may study the variances of the selected model.

Select the model(s) you want to use and click Select to return to the main dialog. Else click Cancel to return to the main dialog without selecting any model.

Text Warning List Dialog

This dialog is accessed by clicking Warnings from the **Get Model** dialog.

Dialog: Text Warning List



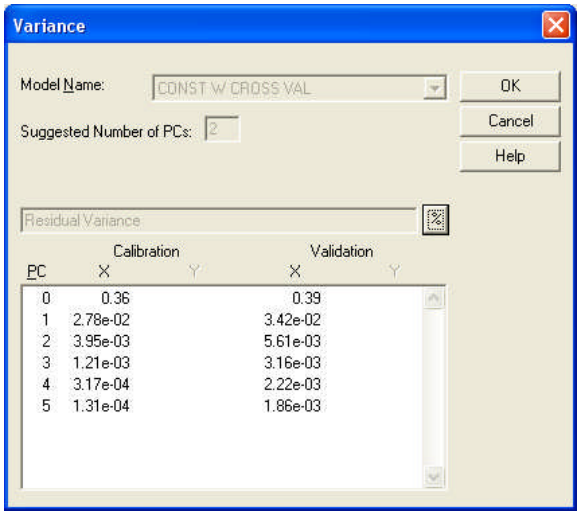
If you want more details, click Outliers; this will display the complete outlier list.

Else just click Close to go back to the main dialog.

Variance Dialog

This dialog is accessed by clicking Variance from the **Classification** dialog, the **Prediction** dialog or the **Get Model** dialog.

Dialog: Variance



The relevant variances (X / Y, Cal / Val) are displayed for each PC. Click the % button if you want to switch from absolute values to percentages. Click OK or Cancel to go back to the main dialog.

Task - Predict...

This task allows you to predict response values from a regression equation.

Depending on the nature of the data table displayed in the Editor upon choosing **Task - Predict**, the following dialog is accessed:

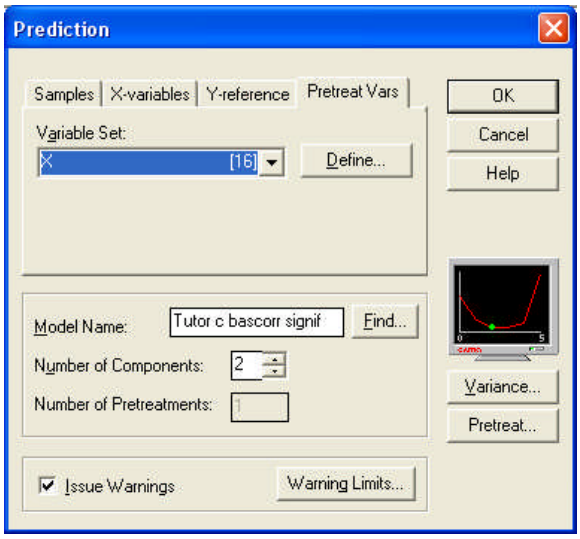
- For a regular (2-D) data table, the **Prediction** dialog shown hereafter allows you to use a regression model of type PLS1, PLS2 or PCR;

- For a 3-D data table, the **Prediction (Three Way PLS)** dialog allows you to use a tri-PLS (nPLS) regression model. This dialog is described in section Prediction (Three Way PLS) Dialog.

Note: What follows applies to 2-D data only.

The **Prediction** dialog contains four sheets: ***Samples***, ***X-variables***, ***Y-reference***, ***Pretreat Vars***, as well as some ***general options*** at the bottom.

Dialog: Prediction



Prediction Dialog: Samples Sheet

Choose which samples to use in your calculation in the Sample Set field and enter any samples which you do not want to include in the analyses in the Keep Out of Calculation field.

For more details, you may lookup the description of a similar dialog in Statistics Dialog: Samples Sheet p.253.

Prediction Dialog: X-variables Sheet

First, choose which Variable Set to use as X for prediction in the Variable Set field. To define new variable sets, click Define to go to the **Set Editor**.

If some of the X-variables were kept out from the model at the calibration stage, they will automatically be kept out at the prediction stage and their numbers will be displayed in the grayed-out field Keep Out of Calculation. This applies once you have selected the model to use (see Prediction Dialog: General Options).

Prediction Dialog: Y-reference Sheet

Tick Include Y-Reference on this sheet if you have reference measurements that you want to use in the prediction. This will activate the Variable Set field, where you specify which set to use as Y-reference either by choosing an existing Variable Set from the drop-down list or by defining a new in the **Set Editor**, which you enter by clicking Define.

These reference values are used only as a comparison, to assess the ***quality*** of the predictions, not to guide the predictions.

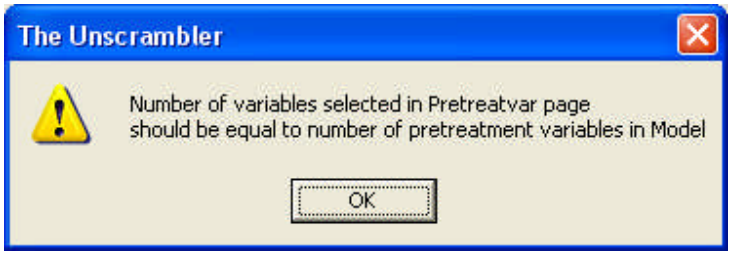
Prediction Dialog: Pretreat Vars Sheet

This sheet is useful if you want to perform automatic pretreatments at prediction. Note that this option is only available if your model has been calibrated on data pretreated in the Unscrambler.

Once you have selected relevant automatic pretreatments using the Pretreat button (see Prediction Dialog: General Options), specify which Variable Set to pretreat, either by choosing an existing Variable Set from the drop-down list or by defining a new in the **Set Editor**, which you enter by clicking Define.

Note: You are free to select a Variable Set to pretreat which differs from the X-Variables set. But make sure that it contains the same number of variables as the original set of variables pretreated prior to building the model. If not, you will get an error message as shown below.

Dialog: Invalid number of Pretreatment Variables


The Unscrambler
Number of variables selected in Pretreatvar page
should be equal to number of pretreatment variables in Model
OK

Prediction Dialog: General Options

You select the model to use in the prediction by entering the model name in the Model Name field or by pressing the Find button next to it to enter the **Get Model** dialog. The number of X-variables in the prediction data set must be the same as the number of X-variables used to build the model. Specify how many PCs to use in the prediction with the spin button.

Press Variance to inspect the calibration and validation variances of the selected model. This takes you to the **Variance** Dialog, where the variances are shown for each PC in the selected model. Toggle between residual and explained variance by pressing the % button.

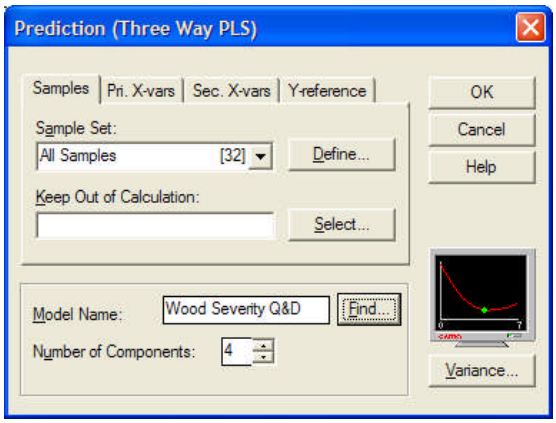
Use the Pretreat button to pretreat the model; this takes you to the **Select transformations** Dialog, where you may choose one or several of the pretreatments that were applied to the calibration data prior to building the regression model your predictions will be based upon. For an explanation of the abbreviations referring to various transformations, see the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

Finally, define whether warnings should be issued by ticking or un-ticking the Issue Warnings box. Ticking it will enable the Warning Limits button, which launches the **Warning Limits** dialog.

Prediction (Three Way PLS) Dialog

The **Prediction (Three Way PLS)** dialog contains four sheets: ***Samples***, ***Pri. X-vars***, ***Sec. X-vars***, ***Y-reference***, as well as a ***Model field*** at the bottom.

Dialog: Prediction (Three Way PLS)



The top of the dialog lets you specify which Sample and Variable Sets to use on the Samples, Pri. X-vars, Sec. X-vars and Y-Variables sheets respectively.

The bottom of the dialog allows you to locate a relevant tri-PLS model and to select the proper number of components for prediction.

Note: Automatic Pretreatment is not available in three-way PLS prediction.

Prediction (Three Way PLS) Dialog: Samples Sheet

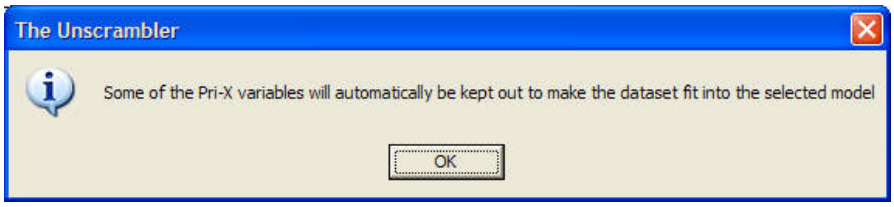
Choose which samples to use in your calculation in the Sample Set field and enter any samples which you do not want to include in the analyses in the Keep Out of Calculation field.

For more details, you may lookup the description of a similar dialog in Statistics Dialog: Samples Sheet p.253.

Prediction (Three Way PLS) Dialog: Pri. X-vars Sheet

Choose which Variable Set to use as Primary X for prediction in the Variable Set field. To define new variable sets, click Define to go to the **Set Editor**.

If some of the Primary X-variables were kept out from the model at the calibration stage, they will automatically be kept out at the prediction stage and their numbers will be displayed in the grayed-out field Keep Out of Calculation. This occurs when you select the model to use (see Prediction (Three Way PLS) Dialog: Model). The following warning will then be displayed:

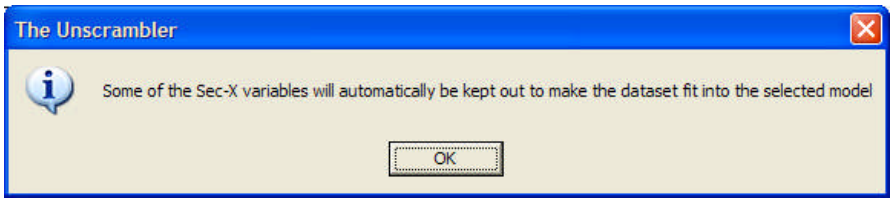

The Unscrambler
Some of the Pri-X variables will automatically be kept out to make the dataset fit into the selected model
OK

Prediction (Three Way PLS) Dialog: Sec. X-vars Sheet

Choose which Variable Set to use as Secondary X for prediction in the Variable Set field. To define new variable sets, click Define to go to the **Set Editor**.

If some of the Secondary X-variables were kept out from the model at the calibration stage, they will automatically be kept out at the prediction stage and their numbers will be displayed in the grayed-out field

Keep Out of Calculation. This occurs when you select the model to use (see Prediction (Three Way PLS) Dialog: Model). The following warning will then be displayed:


The Unscrambler
Some of the Sec-X variables will automatically be kept out to make the dataset fit into the selected model
OK

Prediction (Three Way PLS) Dialog: Y-reference Sheet

Tick Include Y-Reference on this sheet if you have reference measurements that you want to use in the prediction. This will activate the Variable Set field, where you specify which set to use as Y-reference either by choosing an existing Variable Set from the drop-down list or by defining a new in the **Set Editor**, which you enter by clicking Define.

These reference values are used only as a comparison, to assess the ***quality*** of the predictions, not to guide the predictions.

Prediction (Three Way PLS) Dialog: Model

You select the model to use in the prediction by entering the model name in the Model Name field or by pressing the Find button next to it to enter the **Get Model** dialog. The number of Primary and Secondary X-variables in the prediction data set must be the same as the number of Primary and Secondary X-variables used to build the model. Specify how many PCs to use in the prediction with the spin button.

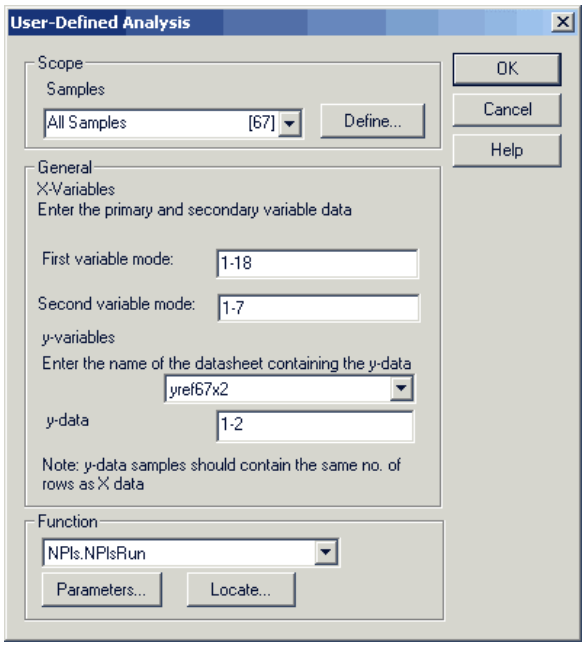
Press Variance to inspect the calibration and validation variances of the selected model. This takes you to the **Variance** Dialog, where the variances are shown for each PC in the selected model. Toggle between residual and explained variance by pressing the % button.

Task - User-defined Analysis

This option has been developed at the request of a group of users who wanted to run their own analyses on 3-D data. It works in a similar way to UDT's.

The option starts the **User-Defined Analysis** (UDA) dialog, where you can specify the scope of the analysis: samples, X-variables of the primary and secondary type, and Y-variables (which have to be stored into another data table where the 3-D structure is not used).

The User-Defined Analysis dialog



The analysis to be performed should be stored in a UDA file that you have previously installed on your computer (See the User Defined Transformations section in the Technical References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices , for a detailed description of how this works). Use Locate… to select your UDA from the list. If it does not appear in the list of available UDT's and UDA's, use Register to register it.

Task - Recalculate with Marked…

Makes a model on only the objects (samples or variables) that you have marked in a given plot. The model parameters are the same as in the model used to make the result plot where you marked these objects.

That means, for instance, that if the plot shows the results of a PCA, a new PCA will be run on only the marked objects. In the **PCA** dialog, the list of unmarked objects is automatically displayed in the Keep Out of Calculation field.

The command can be used for marked samples, for marked X-variables and/or for marked Y-variables.

Note1: The recalculate function applies to the samples or variables marked in the ***currently active plot***. If you wish to select samples, make sure that the active plot contains marked samples. If you wish to select variables, make sure that the active plot contains marked variables.

Note2: In regression results, when using this option from any active variable plot the following rules apply:

- If only some X-variables are marked, the **Recalculate With Marked** option runs a new model including only the marked X-variables and all Y-variables.
- If only some Y-variables are marked, the **Recalculate With Marked** option runs a new model including only the marked Y-variables and all X-variables.
- If both some X-variables and some Y-variables are marked, the **Recalculate With Marked** option runs a new model including all marked variables and excluding all unmarked variables.

Task - Recalculate without Marked…

Makes a model on all objects (samples or variables) other than the ones you have marked in the plot. The model parameters are the same as in the model used to make the result plot where you marked these objects.

That means, for instance, that if the plot shows the results of a PCA, a new PCA will be run excluding all marked objects. In the **PCA** dialog, the list of marked objects is automatically displayed in the Keep Out of Calculation field.

The command can be used for marked samples, for marked X-variables and/or for marked Y-variables.

Note: The recalculate function applies to the samples or variables marked in the ***currently active plot***. If you wish to remove some samples, make sure that the active plot contains marked samples. If you wish to remove some variables, make sure that the active plot contains marked variables.

Task - Recalculate with Passified Marked…

Use this option when you have marked some X- or Y-variables on a Variable plot (e.g. loadings, regression coefficients…) and want the marked variables to be passified in the next analysis. You will then enter the Regression dialog, where the new weights for the variables to be passified will have been updated automatically.

This option is available whenever you have some ***marked X- or Y-variables*** (or both) on the ***currently active plot***. It is not available if you have some marked samples on the currently active plot.

Task - Recalculate with Passified Unmarked…

Use this option when you have marked the important X- and/or Y-variables on a Variable plot (e.g. by using **Edit - Mark - Significant X-variables only**) and want the remaining variables to be passified in the next analysis. You will then enter the Regression dialog, where the new weights for the variables to be passified will have been updated automatically.

This option is available whenever you have some ***marked X- or Y-variables*** (or both) on the ***currently active plot***. It is not available if you have some marked samples on the currently active plot.

If the currently active plot contains only X-variables, the Y-variables will not be affected. If it contains variables of both types, make sure to mark all the variables (X and Y) you want to keep active in your model!

Task - Extract Data from Marked…

Extracts data from the marked objects in the plot and displays them in an Editor window.

Task - Extract Data from Unmarked…

Extracts data from all objects other than the ones you have marked and displays them in an Editor window.

The Results Menu

Results - All…

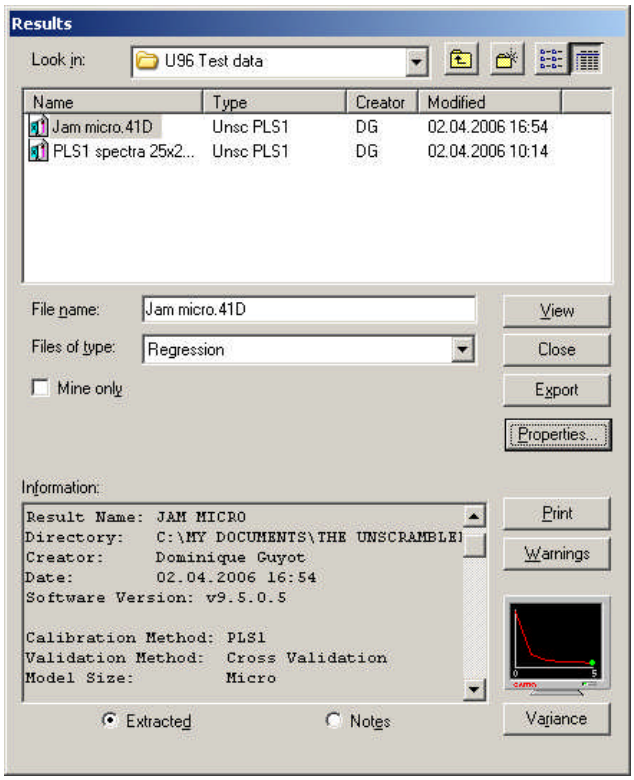
This command launches the **Results** dialog, which gives you an overview of all your data and results files.

The dialog is configured to display Unscrambler files of all types.

Results Dialog

:The **Results** dialog gives you an overview of your data and/or results files, together with some useful buttons.

Dialog: Results



Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

To view only a filtered list of files, select the appropriate type (e.g. ***Regression***) from the drop-down list in the Files of type field.

All files of the selected type, located in the current directory, will be shown. If necessary, click your way to another directory by using the tools at the top of the dialog box.

Tick the box Mine only if you want to filter out files created by other users than yourself.

A regression model can be exported directly from this dialog by pressing the Export button.

Click the Properties button if you want to review the model properties. This also allows you to register transformations for automatic pre-treatment (PCA and Regression models only) by accessing the **Transformations** sheet of the **Properties** dialog.

The Information field at the bottom of the dialog displays information about the selected file. Press Print to get a printout of the information.

Pressing the Warnings button gives you an overview of the warnings that were issued during the given analysis (displayed in the **Text Warning List** dialog).

Pressing the Variance button launches a table of the model variances (displayed in the **Variance** dialog).

If you have chosen a file of type Designed Data, the Warnings button is replaced with a Lab Report button, allowing you to pre-view and print the lab report for the design.

Press Close to exit the dialog without viewing any file.

Results - PCA...

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type PCA.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Regression...

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type Regression.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Response Surface...

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type Response Surface.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Analysis of Effects…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type Analysis of Effects.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Statistics…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **Statistics**.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Classification…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **Classification**.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - Prediction…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **Prediction**.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - MCR...

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **MCR**.

Select the file you wish to view and press View to open a Viewer window where the results will be displayed.

Results - MSC/EMSC…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **MSC**.

You may take advantage of this function to browse through the existing MSC/EMSC model files and check the parameters of a given MSC/EMSC model.

Select the file you wish to view and read the file properties, including the parameters of the MSC transformation, from the Information field. You may press Print to print out the file properties.

Note: MSC/EMSC model files cannot be opened in a Viewer so clicking View will result in an error message.

Results - Data Table…

This command launches the **Results** dialog, which gives you an overview of all your data and results files (see detailed description p.289).

The dialog is configured to display Unscrambler files of type **All Data**.

You may take advantage of this function to browse through the existing data files and check their properties, print them out or print out a Lab Report.

However, data files cannot be opened in a Viewer so clicking View will result in an error message.

Results - General View…

This command launches an empty Viewer where you can make general plots such as a line plots, matrix plots, etc. This option gives you full flexibility in plotting the different results you have made, including results that are not available as predefined model plots.

In the General View, select **Plot** on the Menu Bar and select which kind of plot you want to make. This will launch a plot dialog, where you must specify which data or result file you want to plot samples / variables from.

Details:

- **Plot - Line**: Plot one vector at a time as line, see p. 211
- **Plot - 2D Scatter**: Plot 2 vectors against each other, see p. 212
- **Plot - 3D Scatter**: Plot 3 vectors against each other, see p. 213
- **Plot - Histogram**: Plot one vector as histogram, see p. 214
- **Plot - Matrix**: Plot one or several vectors together as matrix (landscape, contour etc.), see p. 215
- **Plot - Normal Probability**: Plot one vector as N-plot, see p. 215

The Window Menu

Window - Copy To

This option copies the plot in the ***current*** sub-view (***source***) into another sub-view (***destination***).

Seven different sub-views are available; each of them may have some contents even though only a maximum of four are displayed at the same time. The sub-views are organized into three sub-view systems:

1. One sub-view: the Viewer window contains only one sub-view (***number 1***) which uses the ***whole*** window space;
2. Two sub-views: the Viewer window is divided into two horizontal sub-views (***numbers 2 and 3***), each of which uses exactly ***one half*** of the window space;
3. Four sub-views: the Viewer window is divided into four sub-views (***numbers 4 to 7***), each of which uses exactly ***one quarter*** of the window space.

Select which sub-view you want to copy to by choosing a number. The relationship between the numbers and the sub-view layout is shown below.

Relationship between numbers and sub-view layout

Sub-view	Layout	Sub-view	Layout
1		4	
2		5	
3		6	
		7	

As a result of this operation, the destination sub-view becomes active (i.e. current sub-view); the source sub-view retains its plot but is no longer active.

Note: **Copy To** erases the contents of the destination window.

Window - Go To

With this option you can go to a new sub-view and select this as the current sub-view (i.e. activate it).

If you are currently displaying 4 sub-views, Go To - 4 (or 5, 6, 7) is strictly equivalent to clicking into sub-view 4 (or 5, 6, 7).

Use **Go To** when you want to ***change*** your current ***sub-view system***, for instance go from four sub-views to two sub-views.

Seven different sub-views are available; each of them may have some contents even though only a maximum of four are displayed at the same time. The sub-views are organized into three sub-view systems:

4. One sub-view: the Viewer window contains only one sub-view (***number 1***) which uses the ***whole*** window space;
5. Two sub-views: the Viewer window is divided into two horizontal sub-views (***numbers 2 and 3***), each of which uses exactly ***one half*** of the window space;
6. Four sub-views: the Viewer window is divided into four sub-views (***numbers 4 to 7***), each of which uses exactly ***one quarter*** of the window space.

Select which sub-view you want to copy to by choosing a number. The relationship between the numbers and the sub-view layout is shown below.

Relationship between numbers and sub-view layout

Sub-view	Layout	Sub-view	Layout
1		4	
2		5	
3		6	
		7	

Note: **Go To** does not erase the contents of the destination window.

Window - Full Screen

Enlarges the current plot to fill the entire screen. Clicking inside the current plot while holding down the <Shift> key has the same effect.

You can return to normal view by clicking the left mouse button, or by pressing <ESC> or <Enter>.

Note1: For table plots (numeric plots), Full Screen can be activated by using SHIFT-click on the area containing the plot header (at the top of the plot), and de-activated by clicking on the same area.

Note2: Use of **Full Screen** and **Copy To - 1**:

- **Full Screen** blows up the plot to the full size of your physical screen, no matter which space your Viewer window occupies. This is a transitory state; browser info and object info are NOT available.
- **Copy To - 1** copies the plot to the one-sub-view system; the new size of the plot will be that of the Viewer window. This is the largest you can achieve while retaining the browser info and object info capabilities.

Window - Cascade

This option arranges all open windows so that their title bars are visible. To make one the current window, simply click its title bar.

Window - Tile Horizontally

This option sizes and arranges all open windows above each other, so that all are visible. All windows have a “horizontal” layout (wide and short).

Window - Tile Vertically

This option sizes and arranges all open windows side by side, so that all are visible. All windows have a “vertical” layout (tall and thin).

Window - Close Current

Ctrl+F4

Closes the file displayed in the current Editor or Viewer window. If you have made any changes since the last time you saved the file, you are prompted to save the contents before it is closed.

Window - Close All

This option closes all open windows, returning you to The Unscrambler's default opening screen. If you have made any changes in some of the files displayed in those windows, you are prompted to save the contents before the corresponding windows are closed.

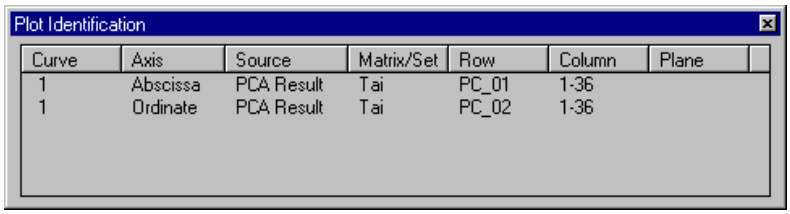
Window - Identification

This is a toggle option which exists for Viewer windows only.

Click it to activate an extra, ***dockable window*** at the bottom of the screen which shows object ***identification of the data in the active plot***. Each data source is described: various curves plotted in a line plot, axes of a 2D-scatter plot, etc.

Together with the **Plot ID** this gives you a good overview of the data contents of the current sub-view.

Identification window

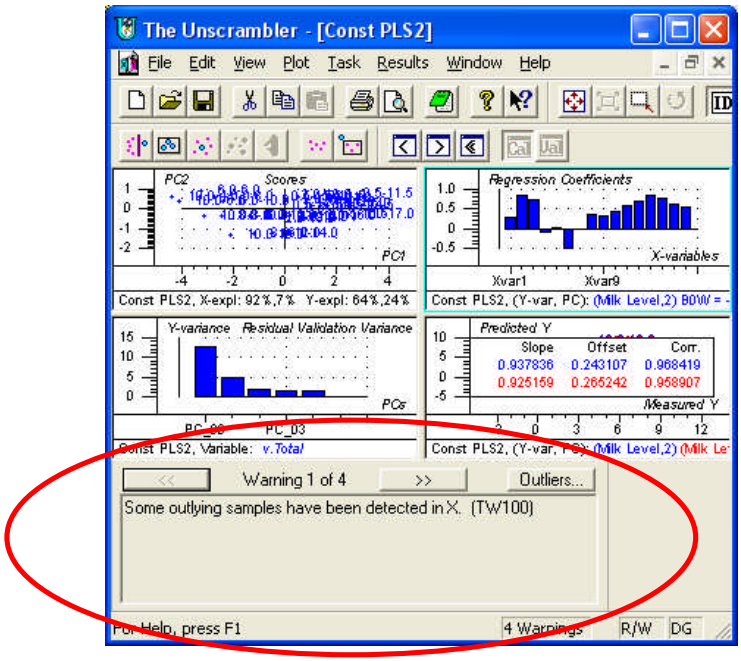


By default, the identification window is ***docked*** to the bottom of the Unscrambler workspace. You may drag it with the mouse and move it around. Drop it somewhere inside the workspace and it will ***float*** over the Viewer as a standalone window.

Window - Warning List

This toggle option available in a result Viewer window shows or hides a list of all the warnings that The Unscrambler generated during computation of the analysis. The list is displayed in a ***dockable window***. These warnings are given in plain English and derive from the thousands of tests that were performed during the model computations.

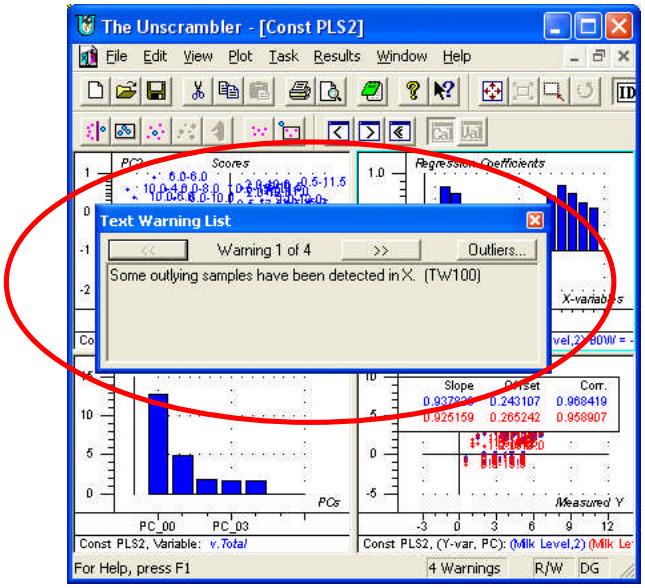
The Unscrambler with the Warning List displayed as docked window at the bottom



Press Outliers to look at a list of the tests that were positive. The outlier list gives a detailed view of the outlier and leverage detection tests.

By default, the warning list window is ***docked*** to the bottom of the Unscrambler workspace. You may drag it with the mouse and move it around. Drop it somewhere inside the workspace and it will ***float*** over the Viewer as a standalone window.

The Unscrambler with the Warning List displayed as a standalone window



Shift to Other Window (1,2…)

This option lets you switch between all currently open windows.

A list at the bottom of the Window menu shows all open document windows, identified with the name of the data or result file displayed in each window.

By clicking at one of the names the window in question will be activated. The list is sorted in historical opening order (first opened window at the top, latest opened window at the bottom of the list).

The Help Menu

Help - The Unscrambler Help Topics

This option opens the Help system on the **Contents** tab.

The Help window is divided into two halves. The Main Help window displays a Help page. The leftmost window contains the Table of Contents, the Index and the Search engine.

Reading the Help System as a Book

You can scan the Help system as a book by clicking your way through the chapters and sections. Either access a chapter directly from the table of contents displayed to the left (use **+** to open sub-chapters) or move up or down, forward or back with the top buttons.

Read more about how to navigate and operate the Help system in the details hereafter.

The Unscrambler Help Toolbar

The Unscrambler Help toolbar

1. The Hide button hides the leftmost window; then only the current Help page is displayed. When the leftmost window is hidden, the Hide button is replaced by Show; hit this if you want the leftmost window to be displayed.
2. The Previous and Next buttons apply to pages that are located just before (Previous) or just after (Next) the currently displayed page in the Help "book".
3. Back takes you one step back in the path that you have followed when reading the Help system. For instance if you follow a link to a new page, hit Back to go back to the page where you clicked on the link. You may then hit Forward if you wish to display the linked page once again, etc.
4. The Print button brings up a dialog where you can choose between printing out:

- only the current chapter, displayed in the main Help window
- or the chapter which is ***currently selected in the table of contents*** + all its sub-chapters.

The Contents, Index and Search Sheets

The leftmost window consists of three sheets: Contents, Index, Search. The tabs let you select which sheet to display.

Contents

This tab opens the Table of Contents, which is the default sheet. Click your way through the main chapters. Display more levels ("open" a chapter) by clicking on "+" or "close" a chapter by clicking on "-".

Index

The Index tab lets you access the Index, where you can search for alphabetically indexed topics.

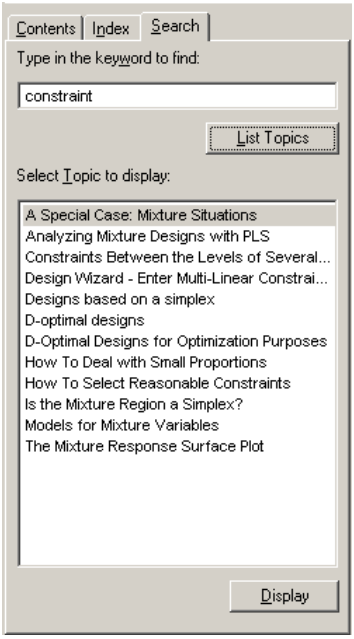
This may be useful for instance in the following cases:

1. Direct access to a ***menu option*** which you want to lookup. Type in the name of the menu, e.g. "file", and under the word "file" in the list of topics you will find all the options that belong to the **File** menu.
2. ***Locate a function*** whose name you are not sure of. You may need to try several keywords before succeeding; be imaginative, do not give up!

Search

The powerful search engine allows you to search for occurrences of one or several words. Once you click on the List Topics button, a list of all Help pages containing the selected word(s) is displayed as shown hereafter.

Finding topics containing the word "constraint"



The page you select from the list is displayed in the main Help window.

Help Button

Gives you help about any component of The Unscrambler.

To use the Help button, click on it – this will activate the button and you will see the shape of the cursor change to an arrow with a question mark.

Move the cursor around and let it rest on the part of The Unscrambler you want help about. Left-clicking on an object will give you specific help about that object, as detailed in the table below.

When Help button is activated, click on… to get help on…

Area you click on	Gives you Help about
Menu option	The corresponding command
Toolbar button	The corresponding command
Plot in the Viewer	Plot interpretation (similar to <F1>)
Other parts of the program	The corresponding feature (e.g. "The Workspace") or the table of contents

Help - Tutorial Exercises

Starts the Tutorials that guide you through several application examples.

How to Use the Tutorials

Each tutorial starts with a presentation of the application example. Read carefully so as to understand the context of the application and the nature of the data.

The next chapters of the tutorial are devoted to practical tasks. The "**Task**" section presents the task in a few words; section "**How To Do It**" gives you detailed instructions:

- Which commands to use;
- How to select correct options in the dialogs;
- How to interpret the results displayed on screen.

Optimize your Windows

The text of the tutorial is displayed in the **Main Help window**. This window, by default, ***floats over*** the Unscrambler workspace. You may re-size both windows and move them around so as to display the tutorial instructions and the Unscrambler workspace ***side by side***.

How To Display Illustrations

Once in a while you will encounter an enhanced text looking like this:

Image link

Display Image A003

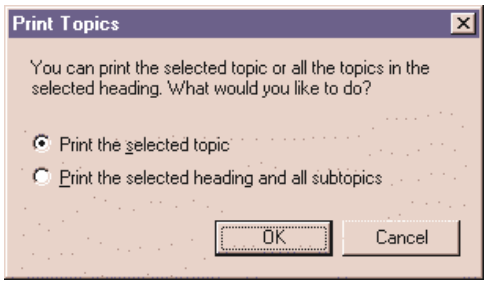
Clicking on this image link will open a **Secondary Help window** where the corresponding illustration is displayed. This secondary Help window can be re-sized and moved around so as to allow you to read the text of the tutorial and look at the illustration simultaneously. If you click either on the Unscrambler workspace or the main Help Window, the image will be ***hidden behind***.

If you want the system to ***remember the size and position*** of the secondary Help window, do not close it; it will simply be updated and appear in front again each time you click on a new image link.

How To Print Out Instructions and Illustrations

From the toolbar at the top of the main Help window, click on the Print icon. This brings up the **Print Topics** dialog.

Dialog: Print Topics


Print Topics
You can print the selected topic or all the topics in the selected heading. What would you like to do?
Print the selected topic
Print the selected heading and all subtopics
OK
Cancel

Choose "Print the selected topic" if you want to print out only the instructions for the ***current task***.

If you wish to print out the instructions for the ***whole tutorial***, go to the first page of the tutorial (e.g. "A Simple Example of Calibration (Tutorial A)") then click on the

icon. From the **Print Topics** dialog, choose "Print the selected heading and all subtopics".

Illustrations can be printed out one at a time by right-clicking anywhere in the secondary Help window where the image is displayed, and selecting **Print…**.

Else you may print out ***all illustrations for a given tutorial*** by downloading a .PDF file containing the tutorial illustrations from CAMO's web pages www.camo.com/TheUnscrambler/Appendices .

Help - Quick Tour

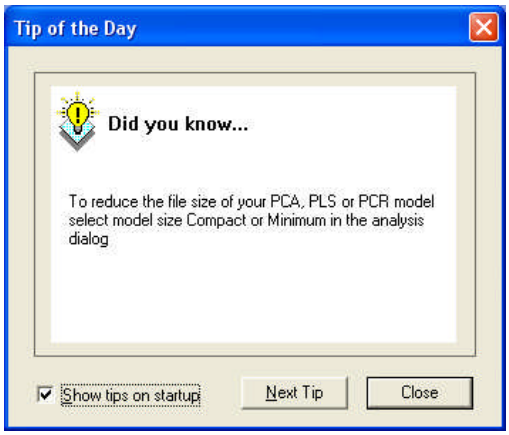
Starts a self-running demo of The Unscrambler.

You may choose among several application examples; the demo presents the application then shows you how the project is run using The Unscrambler. An arrow shows you which menu options are used when running analyses. Main results are presented as plots with comments showing how they were interpreted.

Help - Tip of the Day…

Starts a dialog box where a randomly selected "tip" is displayed.

Dialog: Tip of the Day


Tip of the Day
Did you know...
To reduce the file size of your PCA, PLS or PCR model select model size Compact or Minimum in the analysis dialog
Show tips on startup
Next Tip
Close

Below the text window, a tick-box Show tips on startup allows you to enable / disable the Tip of the Day function on startup.

Use the Next Tip button if you want to browse through the tips database, Close to close the dialog box.

Help - About

Tells you which version of The Unscrambler you are using and copyright notices.

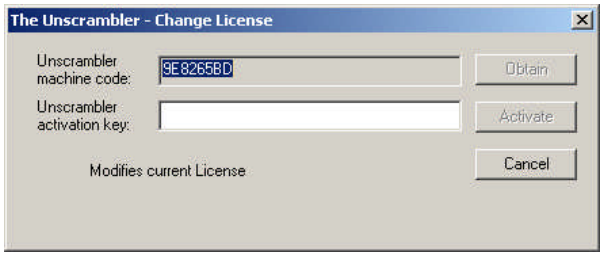
Press Licensee to see who the licensee is and to get information regarding the number of registered and simultaneous users.

Help - Change License

The **Change License** dialog allows you to modifying your current license of The Unscrambler by typing in a new activation key.

Use this feature for instance to upgrade from a trial installation to a full version of The Unscrambler.

Dialog: Change License



Note: This command is only available when logged in as Supervisor.

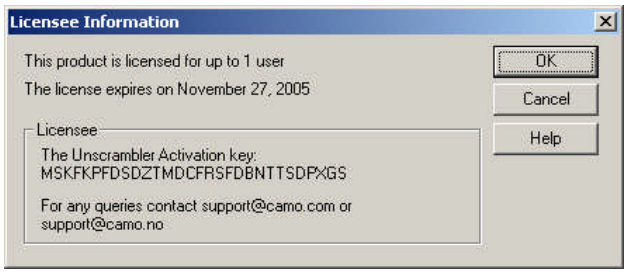
To log in as Supervisor, follow the instructions in the System Configuration chapter p. 22.

Help - Licensee

The Licensee field of the **Licensee Information** dialog displays the Activation key which allows you to activate your Unscrambler license. The activation key is uniquely associated to your license and to the machine on which The Unscrambler is installed.

The dialog also tells you how many users can have access to The Unscrambler, i.e. how many you can have registered in the login list, as well as the expiration date of your license.

Dialog: Licensee Information



Contact CAMO if you need to be able to register more users.

Glossary of Terms

2-D Data

This is the most usual data structure in The Unscrambler, as opposed to 3-D data.

3-D Data

Data structure specific to The Unscrambler which accommodates three-way arrays. A 3-D data table can be created from scratch or imported from an external source, then freely manipulated and re-formatted. Note that analyses meant for two-way data structures cannot be run directly on a 3-D data table. You can analyze 3-D X-data together with 2-D Y-data in a Three-Way PLS regression model. If you want to analyze your 3-D data with a 2-way method, duplicate it to a 2-D data layout first.

Additive Noise

Noise on a variable is said to be additive when its size is independent of the level of the data value. The range of additive noise is the same for small data values as for larger data values.

Category Variable

A category variable is a class variable, i.e. each of its levels is a category (or class, or type), without any possible quantitative equivalent.

Examples: type of catalyst, choice among several instruments, wheat variety, etc..

Candidate Point

In the D-optimal design generation, a number of candidate points are first calculated. These candidate points consist of extreme vertices and centroid points. Then, a number of candidate points is selected D-optimally to create the set of design points.

Center Sample

Sample for which the value of every design variable is set at its mid-level (halfway between low and high).

Center samples can be included when all design variables are continuous.

Closure

In MCR, the Closure constraint forces the sum of the concentrations of all the mixture components to be equal to a constant value (the total concentration) across all samples.

Constraint

1) Context: Curve Resolution:

A constraint is a restriction imposed on the solutions to the multivariate curve resolution problem.

Many constraints take the form of a linear relationship between two variables or more:

$$a_1 . X_1 + a_2 . X_2 + ... + a_n . X_n + a_0 >= 0$$

or

$$a_1 . X_1 + a_2 . X_2 + ... + a_n . X_n + a_0 <= 0$$

where X_i are relevant variables (e.g. estimated concentrations), and each constraint is specified by the set of constants $a_0 \ldots a_n$.

2) Context: Mixture Designs: See Multi-Linear Constraint.

Continuous Variable

Quantitative variable measured on a continuous scale.

Examples of continuous variables are:

- Amounts of ingredients (in kg, liters, etc.);
- Recorded or controlled values of process parameters (pressure, temperature, etc.).

Corner Sample

See vertex sample.

Correlation Loadings

Loading plot marking the 50% and 100% explained variance limits. Correlation Loadings are helpful in revealing variable correlations.

Cross Validation

Validation method where some samples are kept out of the calibration and used for prediction. This is repeated until all samples have been kept out once. Validation residual variance can then be computed from the prediction residuals.

In segmented cross validation, the samples are divided into subgroups or “segments”. One segment at a time is kept out of the calibration. There are as many calibration rounds as segments, so that predictions can be made on all samples. A final calibration is then performed with all samples.

In full cross validation, only one sample at a time is kept out of the calibration.

Cube Sample

Any sample which is a combination of high and low levels of the design variables, in experimental plans based on two levels of each variable.

In Box-Behnken designs, all samples which are a combination of high or low levels of some design variables, and center level of others, are also referred to as cube samples.

Design Def Model

In The Unscrambler, predefined set of variables, interactions and squares available for multivariate analyses on Mixture and D-optimal data tables. This set is defined accordingly to the I&S terms included in the model when building the design (**Define Model** dialog).

Design Variable

Experimental factor for which the variations are controlled in an experimental design.

Edge Center Point

In D-optimal and Mixture designs, the edge center points are positioned in the center of the edges of the experimental region.

End Point

In an axial or a simplex-centroid design, an end point is positioned at the bottom of the axis of one of the mixture variables, and is thus positioned on the side opposite to the axial point.

Gap

One of the parameters of the Gap-Segment and Norris Gap derivatives, the gap is the length of the interval that separates the two segments that are being averaged.

Look up Segment for more information.

Histogram

A plot showing the observed distribution of data points. The data range is divided into a number of bins (i.e. intervals) and the number of data points that fall into each bin is summed up.

The height of the bar in the histograms shows how many data points fall within the data range of the bin.

Hotelling T^2 Ellipse

This 95% confidence ellipse can be included in Score plots and reveals potential outliers, lying outside the ellipse. The Hotelling statistic is presented in the Method References chapter, which is available as a .PDF file from CAMO's web site www.camo.com/TheUnscrambler/Appendices .

Intercept

(Also called Offset). The point where a regression line crosses the ordinate (Y-axis).

Interior Point

Point which is not located on the surface, but inside of the experimental region. For example, an axial point is a particular kind of interior point. Interior points are used in classical mixture designs.

Leveled Variable

A leveled variable is a variable which consists of discrete values instead of a range of continuous values.

Examples are design variables and category variables.

Leveled variables can be used to separate a data table into different groups. This feature is used by the Statistics task, and in sample plots from PCA, PCR, PLS, MLR, Prediction and Classification results.

Levels

Possible values of a variable. A category variable has several levels, which are all possible categories. A design variable has at least a low and a high level, which are the lower and higher bounds of its range of variation. Sometimes, intermediate levels are also included in the design.

Leverage Correction

A quick method to simulate model validation without performing any actual predictions.

It is based on the assumption that samples with a higher leverage will be more difficult to predict accurately than more central samples. Thus a validation residual variance is computed from the calibration sample residuals, using a correction factor which increases with the sample leverage.

Note! For MLR, leverage correction is strictly equivalent to full cross-validation. For other methods, leverage correction should only be used as a quick-and-dirty method for a first calibration, and a proper validation method should be employed later on to estimate the optimal number of components correctly.

Limits For Outlier Warnings

Leverage and Outlier limits are the threshold values set for automatic outlier detection. Samples or variables that give results higher than the limits are reported as suspect in the list of outlier warnings.

Lower Quartile

The lower quartile of an observed distribution is the variable value that splits the observations into 25% lower values, and 75% higher values. It can also be called 25% percentile.

MixSum

Term used in The Unscrambler for ”mixture sum”. See Mixture Sum.

Mixture Sum

Total proportion of a mixture which varies in a Mixture design. Generally, the mixture sum is equal to 100%. However, it can be lower than 100% if the quantity in one of the components has a fixed value.

The mixture sum can also be expressed as fractions, with values varying from 0 to 1.

Mixture Variable

Experimental factor for which the variations are controlled in a mixture design or D-optimal mixture design. Mixture variables are multi-linearly linked by a special constraint called mixture constraint.

There must be at least three mixture variables to define a mixture design. See Mixture Components.

Modes

In a multi-way array, a mode is one of the structuring dimensions of the array. A two-way array (standard n x p matrix) has two modes: rows and columns. A three-way array (3-D data table, or some result matrices) has three modes: rows, columns and planes – or e.g. Samples, Primary variables and Secondary variables.

Multi-Linear Constraint

This is a linear relationship between two variables or more. A constraint has the general form:

$$A_1 . X_1 + A_2 . X_2 + \ldots + A_n . X_n + A_0 >= 0$$

or

$$A_1 . X_1 + A_2 . X_2 + \ldots + A_n . X_n + A_0 <= 0$$

where X_i are designed variables (mixture or process), and each constraint is specified by the set of constants $A_0 \ldots A_n$.

A multi-linear constraint cannot involve both Mixture and Process variables.

Non-Negativity

In MCR, the Non-negativity constraint forces the values in a profile to be equal to or greater than zero.

Normal Probability Plot

The normal probability plot (or N-plot) is a 2-D plot which displays a series of observed or computed values in such a way that their distribution can be visually compared to a normal distribution.

The observed values are used as abscissa, and the ordinate displays the corresponding percentiles on a special scale. Thus if the values are approximately normally distributed around zero, the points will appear close to a straight line going through (0,50%).

A normal probability plot can be used to check the normality of the residuals (they should be normal; outliers will stick out), and to visually detect significant effects in screening designs with few residual degrees of freedom.

O^2V

In The Unscrambler, three-way data structure formed of two Object modes and one Variable mode. A 3-D data table with layout O^2V is displayed in the Editor as a "flat" (unfolded) table with as many rows as Primary samples times Secondary samples and as many columns as Variables.

Offset

See Intercept.

OV^2

In The Unscrambler, three-way data structure formed of one Object mode and two Variable modes. A 3-D data table with layout OV^2 is displayed in the Editor as a "flat" (unfolded) table with as many rows as Objects (samples) and as many columns as Primary variables times Secondary variables.

Passified

When you apply the "Passify" weighting option to a variable, it becomes Passified. This means that it loses all influence on the model, but it is not removed from the analysis, so that you can study how it correlates to the other variables, by plotting Correlation Loadings.

Variables which are not passified may be called "active variables".

Passify

New weighting option which allows you, by giving a variable a very low weight in a PCA, PCR or PLS model, to remove its influence on the model while still showing how it correlates to other variables.

PCs

See Principal Component.

Percentile

The X% percentile of an observed distribution is the variable value that splits the observations into X% lower values, and 100-X% higher values.

Quartiles and median are percentiles. The percentiles are displayed using a box-plot.

PLS1

Version of the PLS method with only one Y-variable.

PLS2

Version of the PLS method in which several Y-variables are modeled simultaneously, thus taking advantage of possible correlations or collinearity between Y-variables.

Prediction

Computing response values from predictor values, using a regression model.

To make predictions, you need

- a regression model (PCR or PLS), calibrated on X- and Y-data;

- new X-data collected on samples which should be similar to the ones used for calibration.

The new X-values are fed into the model equation (which uses the regression coefficients), and predicted Y-values are computed.

Primary Sample

In a 3-D data table with layout O^2V, this is the major Sample mode. Secondary samples are nested within each Primary sample.

Primary Variable

In a 3-D data table with layout OV^2, this is the major Variable mode. Secondary variables are nested within each Primary variable.

Principal Component

PC

Principal Components (PCs) are composite variables, i.e. linear functions of the original variables, estimated to contain, in decreasing order, the main structured information in the data. A PC is the same as a score vector, and is also called a latent variable.

Principal components are estimated in PCA and PCR. PLS components are also denoted PCs.

Process Variable

Experimental factor for which the variations are controlled in an experimental design, and to which the mixture variable definition does not apply.

Proportional Noise

Noise on a variable is said to be proportional when its size depends on the level of the data value. The range of proportional noise is a percentage of the original data values.

Random Order

Randomization is the random mixing of the order in which the experiments are to be performed. The purpose is to avoid systematic errors which could interfere with the interpretation of the effects of the design variables.

Reference Sample

Sample included in a designed data table to compare a new product under development to an existing product of a similar type.

The design file will contain only response values for the reference samples, whereas the input part (the design part) is missing (m).

Replicate

Replicates are experiments that are carried out several times. The purpose of including replicates in a data table is to estimate the experimental error.

Replicates should not be confused with repeated measurements, which give information about measurement error.

Response Variable

Observed or measured parameter which a regression model tries to predict.

Responses are usually denoted Y-variables.

Responses

See Response Variable.

RMSEC

Root Mean Square Error of Calibration. A measurement of the average difference between predicted and measured response values, at the calibration stage.

RMSEC can be interpreted as the average modeling error, expressed in the same units as the original response values.

RMSED

Root Mean Square Error of Deviations. A measurement of the average difference between the abscissa and ordinate values of data points in any 2D scatter plot.

RMSEP

Root Mean Square Error of Prediction. A measurement of the average difference between predicted and measured response values, at the prediction or validation stage.

RMSEP can be interpreted as the average prediction error, expressed in the same units as the original response values.

Sample

Object or individual on which data values are collected, and which builds up a row in a data table.

In experimental design, each separate experiment is a sample.

Scaling

See Weighting.

Secondary Sample

In a 3-D data table with layout O^2V, this is the minor Sample mode. Secondary samples are nested within each Primary sample.

Secondary Variable

In a 3-D data table with layout OV^2, this is the minor Variable mode. Secondary variables are nested within each Primary variable.

Segment

One of the parameters of Gap-Segment derivatives and Moving Average smoothing, a segment is an interval over which data values are averaged.

In smoothing, X-values are averaged over ***one segment*** symmetrically surrounding a data point. The raw value on this point is replaced by the average over the segment, thus creating a ***smoothing*** effect.

In Gap-Segment derivatives (designed by Karl Norris), X-values are averaged separately over ***one segment on each side*** of the data point. The two segments are separated by a gap. The raw value on this point is replaced by the difference of the two averages, thus creating an estimate of the ***derivative*** on this point.

Sensitivity to Pure Components

In MCR computations, Sensitivity to Pure Components is one of the parameters influencing the convergence properties of the algorithm. It can be roughly interpreted as how dominating the last estimated primary principal component is (the one that generates the weakest structure in the data), compared to the first one.

The ***higher*** the sensitivity, the ***more*** pure components will be extracted.

Standardization

Widely used pre-processing that consists in first centering the variables, then scaling them to unit variance.

The purpose of this transformation is to give all variables included in an analysis an equal chance to influence the model, regardless of their original variances.

In The Unscrambler, standardization can be performed automatically when computing a model, by choosing 1/SDev as variable weights.

Star Points Distance To Center

In Central Composite designs, the properties of the design vary according to the distance between the star samples and the center samples. This distance is measured in normalized units, i.e. assuming that the low cube level of each variable is -1 and the high cube level +1.

Three cases can be considered:

- The default star distance to center ensures that all design samples are located on the surface of a sphere. In other words, the star samples are as far away from the center as the cube samples are. As a consequence, all design samples have exactly the same leverage. The design is said to be “rotatable”;

- The star distance to center can be tuned down to 1. In that case, the star samples will be located at the centers of the faces of the cube. This ensures that a Central Composite design can be built even if levels lower than “low cube” or higher than “high cube” are impossible. However, the design is no longer rotatable;
- Any intermediate value for the star distance to center is also possible. The design will not be rotatable.

Star Samples

In optimization designs of the Central Composite family, star samples are samples with mid-values for all design variables except one, for which the value is extreme. They provide the necessary intermediate levels that will allow a quadratic model to be fitted to the data.

Star samples can be centers of cube faces, or they can lie outside the cube, at a given distance (larger than 1) from the center of the cube – see Star Points Distance To Center.

Test Samples

Additional samples which are not used during the calibration stage, but only to validate an already calibrated model.

The data for those samples consist of X-values (for PCA) or of both X- and Y-values (for regression). The model is used to predict new values for those samples, and the predicted values are then compared to the observed ones.

Test Set Validation

Validation method based on the use of different data sets for calibration and validation. During the calibration stage, calibration samples are used. Then the calibrated model is used on the test samples, and the validation residual variance is computed from their prediction residuals.

Training Samples

See Calibration Samples.

UDA

See User-Defined Analysis.

UDT

See User-Defined Transformation.

Uncertainty Limits

Limits produced by Uncertainty Testing, helping you assess the significance of your X-variables in a regression model. Variables with uncertainty limits that do not cross the “0” axis are significant.

Uncertainty Test

Martens' Uncertainty Test is a significance testing method implemented in The Unscrambler, which assesses the stability of PCA or Regression results. Many plots and results are associated to the test, allowing the estimation of the model stability, the identification of perturbing samples or variables, and the selection of significant X-variables. The test is performed with Cross Validation, and is based on the Jack-knifing principle.

Unfold

Operation consisting in mapping a three-way data structure onto a "flat", two-way layout. An unfolded three-way array has one of its original modes nested into another one. In horizontal unfolding, all planes are displayed side by side, resulting in an OV^2 layout, with Primary and Secondary variables. In vertical unfolding, all planes are displayed on top of each other, resulting in an O^2V layout, with Primary and Secondary samples.

Unimodality

In MCR, the Unimodality constraint allows the presence of only one maximum per profile.

Upper Quartile

The upper quartile of an observed distribution is the variable value that splits the observations into 75% lower values, and 25% higher values. It can also be called 75% percentile.

User-Defined Analysis

UDA

DLL routine programmed in C++, Visual Basic, Matlab or other. UDAs allow the user to program his own analysis methods and use them in The Unscrambler.

User-Defined Transformation

UDT

DLL routine programmed in C++, Visual Basic, Matlab or other. UDTs allow the user to program his own pre-processing methods and use them in The Unscrambler.

Validation Samples

See Test Samples.

Variable

Any measured or controlled parameter that has varying values over a given set of samples.

A variable determines a column in a data table.

Vertex Sample

A vertex is a point where two lines meet to form an angle. Vertex samples are used in Simplex-centroid, axial and D-optimal mixture/non-mixture designs.

Ways

See Modes.

Weighting

A technique to modify the relative influences of the variables on a model. This is achieved by giving each variable a new weight, ie. multiplying the original values by a constant which differs between variables. This is also called scaling.

The most common weighting technique is standardization, where the weight is the standard deviation of the variable.

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